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☐	L5	100 and L2	1
☐	L4	100 adj3 M and L2	0
☐	L3	ratio with target with test and L2	1
☐	L2	20040086948.pn.	1
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NEWS 3	MAR 16	CASREACT coverage extended
NEWS 4	MAR 20	MARPAT now updated daily
NEWS 5	MAR 22	LWPI reloaded
NEWS 6	MAR 30	RDISCLOSURE reloaded with enhancements
NEWS 7	APR 02	JICST-EPLUS removed from database clusters and STN
NEWS 8	APR 30	GENBANK reloaded and enhanced with Genome Project ID field
NEWS 9	APR 30	CHEMCATS enhanced with 1.2 million new records
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NEWS 12	MAY 01	New CAS web site launched
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NEWS 14	MAY 14	RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS 15	MAY 21	BIOSIS reloaded and enhanced with archival data
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NEWS 17	MAY 21	CA/CAplus enhanced with additional kind codes for German patents
NEWS 18	MAY 22	CA/CAplus enhanced with IPC reclassification in Japanese patents
NEWS 19	JUN 27	CA/CAplus enhanced with pre-1967 CAS Registry Numbers
NEWS 20	JUN 29	STN Viewer now available
NEWS 21	JUN 29	STN Express, Version 8.2, now available
NEWS 22	JUL 02	LEMBASE coverage updated
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NEWS 24	JUL 02	SCISEARCH enhanced with complete author names
NEWS 25	JUL 02	CHEMCATS accession numbers revised
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NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
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=> solub? (s) deuter? (s) water
L1          190 SOLUB? (S) DEUTER? (S) WATER

=> dup rem l1
PROCESSING COMPLETED FOR L1
L2          143 DUP REM L1 (47 DUPLICATES REMOVED)

=> nmr and l2
L3           41 NMR AND L2

=> py>2001 and l2
L4           45 PY>2001 AND L2

=> l2 not l4
L5           98 L2 NOT L4

=> l3 and l5
L6           21 L3 AND L5

=> t ti l6 1-21

L6   ANSWER 1 OF 21     MEDLINE on STN
TI   Novel reactivity of ruthenium alkylidenes in protic solvents: degenerate
     alkylidene proton exchange.

L6   ANSWER 2 OF 21     MEDLINE on STN
TI   Solubility enhancement of a bisnaphthalimide tumoricidal agent, DMP 840,
     through complexation.

L6   ANSWER 3 OF 21     MEDLINE on STN
TI   Conformational analysis of cyclo(2,9)-Ac-QCRSVEGSCG-OH from the C-terminal
     loop of human growth hormone.

L6   ANSWER 4 OF 21  BIOSIS  COPYRIGHT (c) 2007 The Thomson Corporation  on STN
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TI SOLUBILIZATION OF HYDROCORTISONE IN LYOTROPIC LIQUID CRYSTALS.

L6 ANSWER 5 OF 21 BIOSIS COPYRIGHT (c) 2007 The Thomson Corporation on STN
TI MICRODYNAMICAL BEHAVIOR OF BENZENE SOLUBILIZED IN REVERSE MICELLES A STUDY OF DEUTERIUM NMR RELAXATION.

L6 ANSWER 6 OF 21 CAPLUS COPYRIGHT 2007 ACS on STN
TI Multiple deuteration of water-soluble olefinic acids with a [Pd(alizarin monosulfonate)2] catalyst

L6 ANSWER 7 OF 21 CAPLUS COPYRIGHT 2007 ACS on STN
TI Fourier transform-IR and 1H NMR studies on the structure of water solubilized by reverse aggregates of calcium bis(2-ethylhexyl) sulfosuccinate in organic solvents

L6 ANSWER 8 OF 21 CAPLUS COPYRIGHT 2007 ACS on STN
TI Effects of temperature on sorption of water by wheat gluten determined using deuterium nuclear magnetic resonance

L6 ANSWER 9 OF 21 CAPLUS COPYRIGHT 2007 ACS on STN
TI Use of NMR to probe the structure of water at interfaces of organized assemblies

L6 ANSWER 10 OF 21 CAPLUS COPYRIGHT 2007 ACS on STN
TI A proton and carbon-13 NMR study on the state of water solubilized by detergent aggregates in organic solvents

L6 ANSWER 11 OF 21 CAPLUS COPYRIGHT 2007 ACS on STN
TI Deuterium and nitrogen-14 NMR studies of amphiphilic liquid crystals. Effect of solubilization, electrolyte and temperature on water orientation

L6 ANSWER 12 OF 21 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
TI Proton NMR studies on the structure of water in ionic and nonionic water-in-oil microemulsions

L6 ANSWER 13 OF 21 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
TI Thermally induced structural change of D2O-solubilized AOT reversed micelles and base-catalyzed H-D exchange reaction between solubilized D2O deuterium and AOT-(CH)-C-1 proton

L6 ANSWER 14 OF 21 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
TI RECENT ADVANCES IN MOLECULAR AND SUPERMOLECULAR CHARACTERIZATION OF CELLULOSE AND CELLULOSE DERIVATIVES

L6 ANSWER 15 OF 21 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

TI Production of antibiotic WK-6150 by culturing microorganism in medium for accumulation and collection, useful in pharmaceuticals, veterinary drugs and agrochemicals as antibacterial, antihelmintic and insecticidal agents

L6 ANSWER 16 OF 21 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

TI Interleukin-6 attenuator clovaricin - is used for improving cancerous cachexia caused by excess IL-6 formation due to degeneration of cancer e.g. in liver

L6 ANSWER 17 OF 21 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

TI New antitumour cpd. FD-594 - used for controlling cancer cells.

L6 ANSWER 18 OF 21 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

TI New antiviral cpd. AH-135Y - obtd. from Streptomyces albovinaceus number AH-135

L6 ANSWER 19 OF 21 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

TI Determn. of water content in organic and inorganic media - by dissolving sample in heavy water and recording NMR spectrum, at specified pH level

L6 ANSWER 20 OF 21 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

TI New antibiotic YP-0583 I-alpha - prepared by cultivating Actinoplanes microorganism in medium containing bromine cpds.

L6 ANSWER 21 OF 21 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

TI Antibacterial Bu-2349A - produced by aerobic culture of microorganism of Bacillus strain in aqueous nutrient medium

=> d ibib abs l6 1-21

L6 ANSWER 1 OF 21 MEDLINE on STN
ACCESSION NUMBER: 2001404836 MEDLINE
DOCUMENT NUMBER: PubMed ID: 11457052
TITLE: Novel reactivity of ruthenium alkylidenes in protic solvents: degenerate alkylidene proton exchange.
AUTHOR: Lynn D M; Grubbs R H
CORPORATE SOURCE: Arnold and Mabel Beckman Laboratories of Chemical Synthesis, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California 91125, USA.
SOURCE: Journal of the American Chemical Society, (2001 Apr 11) Vol. 123, No. 14, pp. 3187-93.
Journal code: 7503056. ISSN: 0002-7863.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: NONMEDLINE; PUBMED-NOT-MEDLINE
ENTRY MONTH: 200109
ENTRY DATE: Entered STN: 17 Sep 2001
Last Updated on STN: 17 Sep 2001
Entered Medline: 13 Sep 2001

AB A novel organometallic transformation is reported in which the alkylidene protons of water-soluble ruthenium alkylidenes 1 and 2 undergo nondestructive, degenerate exchange with solvent-derived deuterons in perdeuterated protic solvents such as D(2)O and CD(3)OD. Deuterated alkylidene complex (1-D) was isolated from a solution of alkylidene 1 in D(2)O, and the new alkylidene was fully characterized by (1)H, (2)H, (13)C, and (31)P NMR spectroscopy and fast-atom bombardment mass spectroscopy (FAB-MS). The rate of alkylidene proton exchange for this transformation was found to correlate with the bulk dielectric constant of the solvent or solvent mixtures employed. The data support a mechanism for proton exchange involving the dissociation of a chloride ion from the ruthenium metal center. The rate of alkylidene H/D exchange for alkylidene 2 was faster than the rate of exchange for alkylidene 1, demonstrating that relative rates of exchange are influenced by the electron densities at the metal centers of these complexes. Several additional ruthenium alkylidenes were found to undergo analogous alkylidene H/D exchange reactions, including parent alkylidene

(Cy(3)P)(2)Cl(2)Ru=CHPh (3) in CD(2)Cl(2)/CD(3)OD mixtures. These data suggest that this novel reactivity may be general for an entire class of ruthenium alkylidenes provided that protic species are available in solution and that the dielectric constant of the reaction medium is sufficiently high to ionize the halide ligands.

L6 ANSWER 2 OF 21 MEDLINE on STN
ACCESSION NUMBER: 1998177730 MEDLINE
DOCUMENT NUMBER: PubMed ID: 9552305
TITLE: Solubility enhancement of a bisnaphthalimide tumoricidal agent, DMP 840, through complexation.
AUTHOR: Raghavan K S; Nemeth G A; Gray D B; Hussain M A
CORPORATE SOURCE: DuPont Merck Pharmaceutical Company, Experimental Station, Wilmington, Delaware 19880-0400, USA..
raghavk@a1.lldmpc.umc.dupont.com
SOURCE: Pharmaceutical development and technology, (1996 Oct) Vol. 1, No. 3, pp. 231-8.
Journal code: 9610932. ISSN: 1083-7450.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199804
ENTRY DATE: Entered STN: 7 May 1998
Last Updated on STN: 3 Mar 2000
Entered Medline: 29 Apr 1998

AB The purpose of this research was to enhance the aqueous solubility of DMP 840 by complexation with water-soluble and nontoxic agents, and to understand the nature of the interactions involved in complex formation using nuclear magnetic resonance (1H-NMR). The solubility of DMP 840 in water, saline, acetate buffers, and cosolvent mixtures was determined by high-performance liquid chromatography, and the effect of nicotinamide and pyridoxine concentrations on the solubility of DMP 840 was examined by the phase solubility method. 1H-NMR spectra were acquired in deuterated acetate buffer at 400 MHz on a Varian Unity-400 spectrometer. The aqueous solubility of DMP 840 was sensitive to the presence of chloride and acetate anions in solution, and did not improve in the presence of cosolvents. The use of the nontoxic and water-soluble complex-forming agents nicotinamide and pyridoxine, however, resulted in a linear increase in the aqueous solubility of DMP 840 with both ligands. The solubilization appears to be due to formation of 1:1 complexes between DMP 840 and the bioorganic ligands. The complexation constants were 15.57 M-1 for the DMP 840:nicotinamide complex and 13.36 M-1 for the DMP 840:pyridoxine complex. The NMR results indicate that the interaction is a result of vertical or plane-to-plane stacking and the complexation constants were in agreement with that obtained by phase solubility. The results suggest that the aqueous solubility of a poorly water soluble drug substance such as DMP 840 can be significantly enhanced by its complexation with water-soluble and nontoxic agents.

L6 ANSWER 3 OF 21 MEDLINE on STN
ACCESSION NUMBER: 97273363 MEDLINE
DOCUMENT NUMBER: PubMed ID: 9128096
TITLE: Conformational analysis of cyclo(2,9)-Ac-QCRSVEGSCG-OH from the C-terminal loop of human growth hormone.
AUTHOR: Jois D S; Conrad M W; Chakrabarti S; Siahaan T J
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, University of Kansas, lawrence, USA.
SOURCE: The journal of peptide research : official journal of the American Peptide Society, (1997 Jan) Vol. 49, No. 1, pp. 15-22.
Journal code: 9707067. ISSN: 1397-002X.

PUB. COUNTRY: Denmark
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
(RESEARCH SUPPORT, NON-U.S. GOV'T)
(RESEARCH SUPPORT, U.S. GOV'T, NON-P.H.S.)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199707
ENTRY DATE: Entered STN: 24 Jul 1997
Last Updated on STN: 24 Jul 1997
Entered Medline: 17 Jul 1997

AB A 10 amino acid residue cyclic peptide, cyclo(2,9)-Ac-Gln1-Cys2-Arg3-Ser4-Val5-Glu6-Gly7 -Ser8-Cys9-Gly10, from the C-terminal region of human growth hormone (hGH) was synthesized and studied by 2D proton NMR and molecular dynamics (MD) simulations. The solubility of the peptide was low in water; hence, NMR studies were done in two solvent mixtures, water and deuterated dimethyl sulfoxide. NOE-constrained molecular dynamics and MD simulations resulted in major and minor conformers in solution. The major conformer has a type I beta-turn at Gln1-Cys2-Arg3-Ser4 and a loop structure around Glu6-Gly7-Ser8. Comparison of the conformation of this peptide with the peptide fragment 181-190 in the intact hGH protein X-ray crystal structure indicated that the synthetic peptide retains some structural similarity to the intact protein. Since the C-terminal region is important in binding the hGH protein to its receptor, the conformation of the synthetic peptide could be useful in understanding the binding mechanism.

L6 ANSWER 4 OF 21 BIOSIS COPYRIGHT (c) 2007 The Thomson Corporation on STN
ACCESSION NUMBER: 1991:521142 BIOSIS
DOCUMENT NUMBER: PREV199192132602; BA92:132602
TITLE: SOLUBILIZATION OF HYDROCORTISONE IN LYOTROPIC LIQUID CRYSTALS.
AUTHOR(S): GARTI N [Reprint author]; OSTFELD D; GOUBRAN R; WACHTEL E J
CORPORATE SOURCE: CASALI INST APPLIED CHEM, SCH APPLIED SCI TECHNOL, HEBREW UNIV JERUSALEM, 91904 JERUSALEM, ISRAEL
SOURCE: Journal of Dispersion Science and Technology, (1991) Vol. 12, No. 3-4, pp. 321-336.
CODEN: JDTEDS. ISSN: 0193-2691.
DOCUMENT TYPE: Article
FILE SEGMENT: BA
LANGUAGE: ENGLISH
ENTRY DATE: Entered STN: 19 Nov 1991
Last Updated on STN: 20 Nov 1991

AB The solubilization of hydrocortisone (HC) in lamellar liquid crystals (LC) containing monoglyceride laurate (MGL) and water was studied. The maximum capacity of the 70:30 (wt/wt) MGL/water system to solubilize HC has been found to be larger than any other reported solubilization system (such as microemulsions and micelles), and exceeded 1.0 wt%. The systems were tested by polarized light microscopy, small angle X-ray diffraction, differential scanning calorimetry and deuterium NMR. It was found that the addition of HC caused no change in the interplanar spacing of the system, and had no effect on the gel-to-LC transition temperature. However, the solubilization enlarged the quadrupole splitting of the water deuteron. These results suggest that the HC molecules are positioned in the vicinity of, or within, the polar head groups of the monoglyceride.

L6 ANSWER 5 OF 21 BIOSIS COPYRIGHT (c) 2007 The Thomson Corporation on STN
ACCESSION NUMBER: 1988:371240 BIOSIS
DOCUMENT NUMBER: PREV198886055150; BA86:55150
TITLE: MICRODYNAMICAL BEHAVIOR OF BENZENE SOLUBILIZED IN REVERSE MICELLES A STUDY OF DEUTERIUM NMR RELAXATION.
AUTHOR(S): MAITRA A [Reprint author]
CORPORATE SOURCE: DEP CHEM, DELHI UNIV, DELHI, 110 007

SOURCE: Colloids and Surfaces, (1988) Vol. 32, No. 1-2, pp. 149-158.
CODEN: COSUD3. ISSN: 0166-6622.
DOCUMENT TYPE: Article
FILE SEGMENT: BA
LANGUAGE: ENGLISH
ENTRY DATE: Entered STN: 18 Aug 1988
Last Updated on STN: 18 Aug 1988

AB The reorientational motion of benzene solubilized in a water-Aerosol OT-isooctane reverse micellar system has been studied from the quadrupolar relaxation of deuterated benzene. The correlation time of benzene in the complexed state in reverse micelles is longer than that in pure isooctane solution indicating an association of benzene with the surfactant system. This has also been confirmed from the measurements of activation energies of the relaxation processes in these systems.

L6 ANSWER 6 OF 21 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:414551 CAPLUS
DOCUMENT NUMBER: 133:192893
TITLE: Multiple deuteration of water-soluble olefinic acids with a [Pd(alizarin monosulfonate)2] catalyst
AUTHOR(S): Papp, Eva; Banyai, Istvan; Joo, Ferenc
CORPORATE SOURCE: Research Group of Homogeneous Catalysis, Hungarian Academy of Sciences, Debrecen, H-4010, Hung.
SOURCE: Reaction Kinetics and Catalysis Letters (2000), 69(1), 23-30
CODEN: RKCLAU; ISSN: 0304-4122
PUBLISHER: Akademiai Kiado
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Hydrogenations in aqueous systems with the soluble [Pd(alizarin monosulfonate)2] catalyst resulted in extensive deuteration of crotonic, trans-2-pentenoic and itaconic acids regardless of whether the deuterium source was D2 or D2O. Itaconic acid was deuterated up to 3.6 D/methylsuccinic acid. Detailed 1H-and 13C-NMR studies identified six isotopomers of the deuterated methylsuccinic acid product and revealed an important role of the H/D exchange on the catalytically active Pd-intermediate.

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 21 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:146908 CAPLUS
DOCUMENT NUMBER: 132:242259
TITLE: Fourier transform-IR and 1H NMR studies on the structure of water solubilized by reverse aggregates of calcium bis(2-ethylhexyl) sulfosuccinate in organic solvents
AUTHOR(S): Novaki, L. P.; Pires, P. A. R.; El Seoud, O. A.
CORPORATE SOURCE: Instituto de Quimica Universidade de Sao Paulo, Sao Paulo, 05599-970, Brazil
SOURCE: Colloid and Polymer Science (2000), 278(2), 143-149
CODEN: CPMSB6; ISSN: 0303-402X
PUBLISHER: Springer-Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The structure of water solubilized by reverse aggregates of calcium bis(2-ethylhexyl) sulfosuccinate in deuterobenzene and toluene has been probed by Fourier transform-IR and 1H NMR spectroscopies. The νOD band of solubilized HOD (4% D2O in H2O) has been recorded as a function of the

[water]/[surfactant] molar ratio, W/S. Curve fitting of this band showed the presence of a main peak at 2550 ± 13 cm-1 and a small one at 2405 ± 15 cm-1. As a function of increasing W/S, the frequency of the main peak decreases, its full width at half-height increases, and its area increases linearly. The 1H NMR chemical shift of solubilized H2O-D2O mixts. at W/S = 18.1 has been measured as a function of the deuterium content of the aqueous nanodroplet. These data were used to calculate the so-called "fractionation factor" of the aggregate-solubilized water, the value of which was found to be unity. The results of both techniques show that reverse aggregate-solubilized water, although different from bulk water, does not seem to coexist in "layers" of different degrees of structure, as suggested, for example by the two-state water-solubilization model.

REFERENCE COUNT: 73 THERE ARE 73 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 21 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:197843 CAPLUS
DOCUMENT NUMBER: 131:18238
TITLE: Effects of temperature on sorption of water by wheat gluten determined using deuterium nuclear magnetic resonance
AUTHOR(S): Grant, A.; Belton, P. S.; Colquhoun, I. J.; Parker, M. L.; Plijter, J. J.; Shewry, P. R.; Tatham, A. S.; Wellner, N.
CORPORATE SOURCE: Institute of Food Research, Norwich Laboratory, Norwich, NR4 7UA, UK
SOURCE: Cereal Chemistry (1999), 76(2), 219-226
CODEN: CECHAF; ISSN: 0009-0352
PUBLISHER: American Association of Cereal Chemists
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The effects of lipids and residual starch components of wheat flour gluten on gluten hydration properties were investigated using NMR and Fourier transform IR (FT-IR) techniques. Whole or native, lipid-free, starch-free, and lipid- and starch-free gluten samples were prepared from wheat (Triticum aestivum) cv. Mercia. 2H NMR relaxation on gluten samples hydrated with deuterium oxide (D2O) was measured over a 278-363 K temperature range. FT-IR spectra were recorded in dry and fully hydrated material. Transverse relaxation (T2) results indicated that all 4 gluten samples were hydrophilic in nature. There was little difference in relaxation behavior of whole and lipid-free gluten samples. T2 values and populations of the relaxation components were very similar in each. The FT-IR spectra of both samples showed an increase in extended β-sheet secondary structures on hydration. These results suggest that lipid binding in gluten, if it occurs, has little effect on wheat gluten properties. Adding starch to the gluten matrix results in an increase in water sorption on heating that may be attributed to the effects of starch gelation. However, the whole water uptake of the gluten cannot be accounted for by the contribution of the residual starch, as estimated by the effects of added starch. Extraction of residual starch required solubilization of the protein, including breaking of the disulfide bonds. This process altered the gluten structure and properties. Light microscope investigation showed that glutens with residual starch extracted were unable to form fibrillar strands on hydration. NMR and FT-IR results showed greater water sorption in both samples with extracted starch than in the unextd. samples.

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 21 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:456500 CAPLUS
DOCUMENT NUMBER: 127:210588
TITLE: Use of NMR to probe the structure of water at interfaces of organized assemblies
AUTHOR(S): El Seoud, Omar A.
CORPORATE SOURCE: Instituto de Quimica, Universidade de Sao Paulo, C.P. 26.077, Sao Paulo, S.P., 05599-970, Brazil
SOURCE: Journal of Molecular Liquids (1997), 72(1/3), 85-103
CODEN: JMLIDT; ISSN: 0167-7322
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with 58 refs. which addresses the use of NMR spectroscopy to probe the structure of interfacial water of organized assemblies: aqueous micelles, reverse micelles, RMs, and water-in-oil microemulsions, W/O μEs. For aqueous micelles, the dependence of the 1H NMR chemical shift of water on [surfactant] is measured in H2O-D2O mixts. In case of RMs and W/O μEs, one dets. the dependence of 1H NMR chemical shift of solubilized H2O-D2O, and/or 1H and 13C chemical shifts of the surfactant headgroup on the deuterium content of solubilized water. The measured deuterium isotope effect on the appropriate chemical shift is then used to calculate the so called "deuterium/protium fractionation factor, .vphi." for interfacial water. Values of .vphi. thus obtained are rationalized in terms of effects of the interface on the structure of its water of hydration, relative to that of bulk water. The important conclusions of this review are: (1) effects of simple ions (e.g., butylsulfate or butyltrimethylammonium) on the structure of water are different from those of micellized ions (e.g., dodecylsulfate or cetyltrimethylammonium plus the associated counterions), this difference is due to electrostriction of water by the charged interface; (2) perturbation of the structure of interfacial water is larger for ionic micelles than for the corresponding zwitterionic ones; (3) For the same class of surfactants, e.g., cationic or zwitterionic, the micelle-induced enhancement of the structure of interfacial water (relative to that of bulk water) increases as a function of increasing the hydrophobic character of the surfactant headgroup; (4) Water solubilized by RMs and W/O μEs does not seem to coexist in "layers" of different structures within the micellar water "pool".
REFERENCE COUNT: 103 THERE ARE 103 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 21 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:227895 CAPLUS
DOCUMENT NUMBER: 120:227895
TITLE: A proton and carbon-13 NMR study on the state of water solubilized by detergent aggregates in organic solvents
AUTHOR(S): El Seoud, Omar A.; El Seoud, Monica I.; Mickiewicz, Joseph A.
CORPORATE SOURCE: Inst. Quim., Univ. Sao Paulo, Sao Pualo, 01498-970, Brazil
SOURCE: Journal of Colloid and Interface Science (1994), 163(1), 87-93
CODEN: JCISA5; ISSN: 0021-9797
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The state of H2O solubilized by the reversed micelles of the surfactants CTAB and (AOT) in organic solvents was examined by a novel, noninvasive technique based on measuring the dependence of the 1H chemical shift of solubilized H2O, 1H and 13C chemical shifts of the discrete groups of the surfactant on the D content of solubilized H2O, and the

[H2O]/[surfactant], W/S, ratio. Graphs of the chemical shifts vs. the atom fraction of D in the micelle-solubilized H2O were strictly linear (W/S 4-20) and were used to calculate the fractionation factor (ϕ) for solubilized H2O. A value of unity was obtained in all cases, indicating that the structure of the micelle-solubilized H2O is the same over the whole volume of the aqueous nanodroplet (i.e., H2O does not seen to coexist in "layers" of different degrees of structure).

L6 ANSWER 11 OF 21 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:198213 CAPLUS
DOCUMENT NUMBER: 86:198213
TITLE: Deuterium and nitrogen-14 NMR studies of amphiphilic liquid crystals. Effect of solubilization, electrolyte and temperature on water orientation
AUTHOR(S): Persson, Nils Ola; Lindman, Bjorn
CORPORATE SOURCE: Div. Phys. Chem. 2, Chem. Cent., Lund, Swed.
SOURCE: Molecular Crystals and Liquid Crystals (1977), 38(1-4), 327-44
CODEN: MCLCA5; ISSN: 0026-8941
DOCUMENT TYPE: Journal
LANGUAGE: English
AB D NMR on hexagonal and lamellar amphiphile-D2O mesophases was used to study the partial orientation of the water mols. and how the degree of orientation is influenced by solubilization of organic compds., by addition of simple electrolytes and by temperature changes. Solubilization effects follow roughly the polarity of the solubilizate, a more polar solubilizate producing a greater reduction in the degree of water orientation, but important differences exist between -CO2- and -OSO3- end-groups of the surfactant. These results are discussed in terms of changes in amphiphile hydration and altered packing conditions in the aggregates. The effect of electrolyte addition depends markedly on both counterion and co-ion and is discussed on the basis of ion hydration. For Me4N octanoate-D2O system, the degree of water orientation increases with increasing water content, and this may arise from a particular counterion binding mechanism in this case. The counterion binding in this system as well as the NH4 octanoate-D2O system was further studied by means of 14N quadrupole splittings.

L6 ANSWER 12 OF 21 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
ACCESSION NUMBER: 1996:573464 SCISEARCH
THE GENUINE ARTICLE: VA409
TITLE: Proton NMR studies on the structure of water in ionic and nonionic water-in-oil microemulsions
AUTHOR: ElSeoud O A (Reprint); Okano L T; Novaki L P; Barlow G K
CORPORATE SOURCE: UNIV SAO PAULO, INST QUIM, CP 26-077, BR-05599970 SAO PAULO, SP, BRAZIL (Reprint); UNIV YORK, DEPT CHEM, YORK YO1 5DD, N YORKSHIRE, ENGLAND
COUNTRY OF AUTHOR: BRAZIL; ENGLAND
SOURCE: BERICHTE DER BUNSEN-GESELLSCHAFT-PHYSICAL CHEMISTRY CHEMICAL PHYSICS, (JUL 1996) Vol. 100, No. 7, pp. 1147-1152.
ISSN: 0005-9021.
PUBLISHER: VCH PUBLISHERS INC, 303 NW 12TH AVE, DEERFIELD BEACH, FL 33442-1788.
DOCUMENT TYPE: Article; Journal
FILE SEGMENT: PHYS
LANGUAGE: English
REFERENCE COUNT: 58
ENTRY DATE: Entered STN: 1996
Last Updated on STN: 1996

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The structure of water present in water-in-oil microemulsions of anionic magnesium bis(2-ethylhexyl) sulfosuccinate in C6D6, cationic cetyldimethylbenzylammonium chloride in C6D6, cetyldimethyl-3-phenylpropylammonium chloride in chlorobenzene, and nonionic polyoxyethylene (4) dodecyl ether in n-heptane was probed by H-1 NMR. Chemical shifts of solubilized H2O-D2O, and of surfactant discrete protons were determined, at fixed [water]/[surfactant] ratios, as a function of the deuterium content of solubilized water. Chemical shift data were used to calculate the so called ''fractionation factor'', phi, of the aggregate-solubilized water. Calculated phi, for the different systems are unity, showing that micellar water, although different from bulk water, does not seem to coexist in ''layers'' of different degrees of structure, as suggested, e.g., by the two-state water solubilization model.

L6 ANSWER 13 OF 21 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN

ACCESSION NUMBER: 1996:381327 SCISEARCH
THE GENUINE ARTICLE: UL282
TITLE: Thermally induced structural change of D2O-solubilized AOT reversed micelles and base-catalyzed H-D exchange reaction between solubilized D2O deuterium and AOT-(CH)-C-1 proton
AUTHOR: Yoshino A (Reprint); Okabayashi H; Uchida T; Ogasawara T; Yoshida T; OConnor C J
CORPORATE SOURCE: NAGOYA INST TECHNOL, DEPT APPL CHEM, SHOWA KU, NAGOYA, AICHI 466, JAPAN; UNIV AUCKLAND, DEPT CHEM, AUCKLAND 1, NEW ZEALAND
COUNTRY OF AUTHOR: JAPAN; NEW ZEALAND
SOURCE: JOURNAL OF PHYSICAL CHEMISTRY, (16 MAY 1996) Vol. 100, No. 20, pp. 8418-8424.
ISSN: 0022-3654.
PUBLISHER: AMER CHEMICAL SOC, 1155 16TH ST, NW, WASHINGTON, DC 20036.
DOCUMENT TYPE: Article; Journal
FILE SEGMENT: PHYS
LANGUAGE: English
REFERENCE COUNT: 45
ENTRY DATE: Entered STN: 1996
Last Updated on STN: 1996

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The temperature dependence of the H-1 NMR spectrum for the D2O-solubilized Aerosol-OT (AOT)-C6D6 system in the reversed micellar state has been investigated in the temperature range 323-353 K. From the H-1 chemical shift variation of the AOT polar segment protons and of the HDO proton, it has been assumed that a structural transition of water incorporated into the polar core occurs at 343 K and that this transition is the result of the variation in interaction between water molecules within the polar core and those solubilized at or close to polar head groups of the ethylhexyl chains, The base-catalyzed H-D exchange reaction between the AOT-(CH)-C-1 proton and solubilized D2O deuterium has also been investigated in this temperature range. Kinetic analysis, based on the time dependence of the H-1 NMR spectrum, has allowed evaluation of the thermodynamic parameters of the exchange reaction to be made. These show a marked difference between the two temperature ranges 323-343 and 343-353 K. In particular, it has been suggested, from the C-13 chemical shift data, that the local concentration of the OD- anions has a considerable influence on the H-D exchange reaction in the temperature range 323-353 K.

L6 ANSWER 14 OF 21 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN

ACCESSION NUMBER: 1994:414360 SCISEARCH
THE GENUINE ARTICLE: NU648
TITLE: RECENT ADVANCES IN MOLECULAR AND SUPERMOLECULAR CHARACTERIZATION OF CELLULOSE AND CELLULOSE DERIVATIVES
AUTHOR: KAMIDE K (Reprint); SAITO M
CORPORATE SOURCE: KUMAMOTO UNIV, FAC EDUC, CLOTHING LAB, KUROKAMI 2-40-1, KUMAMOTO 860, JAPAN (Reprint); ASAHI CHEM IND CO LTD, FUNDAMENTAL RES LAB NAT & SYNTHET POLYMERS, OSAKA 569, JAPAN
COUNTRY OF AUTHOR: JAPAN
SOURCE: MACROMOLECULAR SYMPOSIA, (MAY 1994) Vol. 83, pp. 233-271. ISSN: 1022-1360.
PUBLISHER: HUTHIG & WEPF VERLAG, AUF DEM WOLF 4 FX#001-41-61-317-94-11, CH-4052 BASEL, SWITZERLAND.
DOCUMENT TYPE: Article; Journal
FILE SEGMENT: PHYS
LANGUAGE: English
REFERENCE COUNT: 37
ENTRY DATE: Entered STN: 1994
Last Updated on STN: 1994

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Recent advances between 1985 and early 1993 in the following topics of the characterization of molecular structure and molecular properties of cellulose and its derivates (CD) made in the authors' laboratories are briefly reviewed: (1) A theoretical basis of the assignment of carbonyl carbon peaks of C-13 NMR spectra on cellulose acetate (CA) was given, especially when the total degree of substitution <<F>> is below 3. (2) Molar fractions of 8 kinds of unsubstituted and partially or fully substituted anhydroglucopyranose units were successfully determined for CA and sodium cellulose sulfate (NaCS). (3) The sequence distribution of substituted and unsubstituted anhydroglucopyranose units along a water-soluble CA chain was evaluated. (4) C6-substituted (i.e., 6-O-acetyl) CA and C2- and C6-substituted CA were synthesized, and the full assignment of the C-13 NMR spectrum of the former was given and a new method for evaluating the degree of substitution at C6 position was proposed. (5) By destructing the intramolecular hydrogen bonding, cellulose becomes soluble in aqueous sodium hydroxide. The specific supermolecular structure of aqueous sodium hydroxide, dissolving mechanism, dissolved state and molecular parameters of cellulose in aqueous sodium hydroxide were discussed. (6) The solubility behavior of CA with a wide range of total degree of substitution in solvents including water, acetone/water and acetone is controlled by the distribution of substitution and the supermolecular structure. (7) The existence of O3-H...O5' intramolecular hydrogen bonds in a water -insoluble cellulose derivative with hydrophilic substituent (NaCEC) was confirmed by CP/MAS C-13 NMR and deuteration IR method. At a relatively low degree of substitution the solubility of the derivative in water or aqueous alkali was mainly governed by considerable destruction of the intramolecular hydrogen bonds. (8) The persistence length q, evaluated directly by small-angle X-ray scattering (SAXS) on CA with different total degree of substitution <<F>> ranging from 0,8 to 2,9 confirmed definitely the conclusion drawn before by Kamide and Saito on the molecular rigidity of CD, especially the effect of <<F>> on q. (9) C6-substituted CA shows different solubility towards dimethylacetemide and water at 20-degrees-C, as compared with C2- and C3-substituted CA and C2-, C3- and C6- substituted CA, whose <<F>> is ca. 0,6.

L6 ANSWER 15 OF 21 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 2001-582057 [65] WPIDS
DOC. NO. CPI: C2001-172576 [65]
TITLE: Production of antibiotic WK-6150 by culturing microorganism in medium for accumulation and collection, useful in pharmaceuticals, veterinary drugs and

agrochemicals as antibacterial, antihelmintic and insecticidal agents
DERWENT CLASS: B02; C02; D16
INVENTOR: IWAI Y; OMURA S; SHIOMI K; TAKAHASHI Y
PATENT ASSIGNEE: (KITA-C) KITASATO INST
COUNTRY COUNT: 83

PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
WO 2001062950	A1	20010830	(200165)*	JA	24[2]	
AU 2000026913	A	20010903	(200202)	EN		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2001062950	A1	WO 2000-JP1064	20000224
AU 2000026913	A	AU 2000-26913	20000224
AU 2000026913	A	WO 2000-JP1064	20000224

FILING DETAILS:

PATENT NO	KIND		PATENT NO
AU 2000026913	A	Based on	WO 2001062950 A

PRIORITY APPLN. INFO: WO 2000-JP1064 20000224
AN 2001-582057 [65] WPIDS
AB WO 2001062950 A1 UPAB: 20050526
NOVELTY - Antibiotic WK-6150 of formula (I) is new.
DETAILED DESCRIPTION - Antibiotic WK-6150 of formula (I) is new.
INDEPENDENT CLAIMS are also included for:
(1) antibiotic WK-6150 with physiochemical properties of being a white powder, having molecular weight of 785.5157 (M+Na by FABMS), molecular formula of C44H74O10, melting point 125-128degreesC, optical rotation, (alpha)D25 = -62.7degrees (c = 0., methanol), UV spectrum in methanol with absorption peaks e.g. at 225 nm (epsilon = 63600), IR spectrum using KBr pressed-disk with maximum absorption peaks at e.g. 2866 and 1701, 1H and 13C NMR spectra in deuteriated acetone (chemical shifts available), and soluble in methanol, acetone and chloroform but sparingly soluble in water; and
(2) a method for producing antibiotic WK-6150 by culturing a microorganism capable of producing the substance in a medium before accumulation and isolation.
ACTIVITY - Antibacterial; antihelmintic; insecticidal.
MECHANISM OF ACTION - None given.
USE - The antibiotic is useful in pharmaceuticals, veterinary drugs and agrochemicals as antibacterial, antihelmintic and insecticidal agents.
ADVANTAGE - Such antibiotic has lower toxicity, side-effects and drug-resistance.

L6 ANSWER 16 OF 21 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 1997-083464 [08] WPIDS
DOC. NO. CPI: C1997-026815 [08]
TITLE: Interleukin-6 attenuator clovaricin - is used for improving cancerous cachexia caused by excess IL-6 formation due to degeneration of cancer e.g. in liver
DERWENT CLASS: B04; D16
INVENTOR: HAYASHI M; KOMIYAMA H; OMURA S; TAKAMATSU S
PATENT ASSIGNEE: (KITA-C) KITASATO KENKYUSHO SH

COUNTRY COUNT: 1

PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 08325284	A	19961210	(199708)*	JA	8[3]	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 08325284 A		JP 1995-128217	19950526

PRIORITY APPLN. INFO: JP 1995-128217 19950526
AN 1997-083464 [08] WPIDS
AB JP 08325284 A UPAB: 20050515
New clovaricin (I) has the following physicochemical properties: (1) colourless oil; (2) mol.weight 332 (determined by FAB-MS); (3) mol. formula: C16H25O5Cl (determined by high resolution mass spectrum); (4) UV/visible absorption spectrum (Fig.1): lambda maximum 205 nm (log epsilon: 3.42), 220 (2.88 sh); (5) solubility: soluble in acetone, EtOAc, Et2O, hexane, MeOH, EtOH, CHCl3 and benzene, sparingly soluble in water; (6) proton-NMR (in deuterated MeOH); (7) 13C-NMR (in deuterated MeOH); and (8) colour reaction: positive to H2SO4, phosphomolybdic acid or iodine.
Also claimed are: (A) production of (I) is incubating clovaricin-producing strain of Sporothrix on a culture medium to accumulate (I) therein and recovering (I) from the culture broth; and (B) clovaricin-producing strain of Sporothrix (specifically: Sporothrix sp. FO-4649 (FERM P-14796).
USE/ADVANTAGE - (I) is used in improvement of cancerous cachexia caused by excess generation of interleukin-6 (IL-6) which is accompanied by degeneration of cancers, e.g. cancer in lung, liver, colon, or prostate. Also effective for multiple myeloma or articular rheumatism. In a test using an IL-6 dependent murine myeloid cell MH-60, (I) inhibited growth of MH-60 as follows: growth rate of MH-60: 0.50% at 12.5 (micro g/ml) of (I), 5.20% at 6.25, 40.5% at 3.13, 74.3% at 1.56, and 102.4% at 0.78.

L6 ANSWER 17 OF 21 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 1996-157089 [16] WPIDS
DOC. NO. CPI: C1996-049273 [16]
TITLE: New antitumour cpd. FD-594 - used for controlling cancer cells.
DERWENT CLASS: B04; D16
INVENTOR: ANDO T; KIYOU A; MIZOGAMI K; MORIMOTO S; OKAZAKI T
PATENT ASSIGNEE: (TAIS-C) TAISHO PHARM CO LTD
COUNTRY COUNT: 1

PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 08041092	A	19960213	(199616)*	JA	7[3]	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 08041092 A		JP 1994-177784	19940729

PRIORITY APPLN. INFO: JP 1994-177784 19940729
AN 1996-157089 [16] WPIDS

AB JP 08041092 A UPAB: 20050511
Anti-tumour active cpd. FD-594 having the following physicochemical properties is new. (1) Appearance: yellow powder. (2) M.pt.: 217-220 deg.C. (3) mass spectroscopy: SIMS spectrum, m/z 941(M+H)(+); SIMS(+KI) spectrum, m/z 979(M+K)(+); anion FABMS spectrum, m/z 939(M=H)(-). (4) FABMS-high-resolution mass spectrum: observed, 979, 9009; theoretical, 979, 2975 (calculated as C43H52N6018K). (5) Molecular formula: C43H52N6O18, (6) Molecular weight: 940. (7) UV absorption spectrum: lambda(epsilon), 206(40700), 235(366000), 276(43800), 300(sh) (28500), 365(21400), 420(6100) nm, in methanol; lambda(epsilon), 206(40700), 215(40600), 235(36700), 276(49000), 300(sh) (32600), 365(23300), 420(6100)nm, in HCl-methanol; lambda(epsilon), 209(93300), 243(43800), 276(36800), 285(sh) (35600), 375(20600), 440(9700) nm, in NaOH-methanol; (8) specific IR absorption spectrum measured in the KBR tablet; (9) specific 1H-NMR spectrum measured at 300 MHz in deuterated chloroform; (10) specific 13C-NMR spectrum measured at 75 MHz in deuterated chloroform; (11) Solubility: soluble in DMSO and pyridine, only slightly soluble in methanol, acetone and chloroform and insol. in water and hexane.

USE/ADVANTAGE - The cpd. is useful as a drug against cancers. The cpd. has growth-controlling effect against cultured cancer cells.

L6 ANSWER 18 OF 21 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 1993-224301 [28] WPIDS
DOC. NO. CPI: C1993-099778 [28]
TITLE: New antiviral cpd. AH-135Y - obtd. from Streptomyces albovinaceus number AH-135
DERWENT CLASS: B02; B03; D16
INVENTOR: AOKI M; KIDO Y; KINO Y; NAKAJIMA K; UEDA M
PATENT ASSIGNEE: (KAGA-N) ZH KAGAKU YOBI KESSEI RYOHO KENKYUSHO
COUNTRY COUNT: 1

PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 05148230	A	19930615	(199328)*	JA	8[0]	
JP 3176672	B2	20010618	(200136)	JA	9	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 05148230 A		JP 1991-340339	19911128
JP 3176672 B2		JP 1991-340339	19911128

FILING DETAILS:

PATENT NO	KIND	PATENT NO
JP 3176672 B2	Previous Publ	JP 05148230 A

PRIORITY APPLN. INFO: JP 1991-340339 19911128
AN 1993-224301 [28] WPIDS
AB JP 05148230 A UPAB: 20050509
Antiviral substance AH-135Y (I) has (1) chemical structure of formula (I); (2) elementary analysis: C 61.8%; H 5.98%, N 4.79%; (3) molecular weight of 291; (4) molecular formula of C15H17NO3; (5) m.pt. of 210-230 deg.C; (6) UV absorption spectrum (in methanol) of lamda max nm (E1%, 1 cm) of 218 (634.8), 259.5 (311.5), 342.5 (138.4); (7) IR absorption spectrum (KBr) of 3510, 1715, 1660, 1270 cm-1; (8) NMR spectrum (deuterized DMSO) of 2.29, 2.39, 2.62, 3.19, 4.51, 5.17, 7.49,

7.65, 10.77, 12.2 ppm; (9) 13C NMR spectrum (deuterized DMSO) of 20.1, 25.9, 36.9, 42.3, 57.1, 118.1, 127.2, 128.3, 130.6, 134.8, 156.2, 172.8, 205.3 ppm; (10) solubility in methanol, ethanol, acetone, ethyl acetate and dimethyl sulphoxide, and partial solubility in benzene, ether, hexane, chloroform and water ; (11) dark greenish colour reaction with alcoholic ferric chloride; (12) thin-layer chromatography; Rf 0.38 (chloroform-acetone= 3:1), 0.085 (hexane-ethyl acetate-methanol-acetic acid=10:5:0:0.5:0.1) on simical gel; and (13) white powder appearance.

Production of an antiviral substance AH-135Y (I) comprises cultivating a (I)-producing microorganism of Streptomyces and recovering (I) from the cultured broth. Suitable strain can be Streptomyces albovinaceus AH-135Y (FERM P-12603).

USE - As antiviral agent. - In an example, one Pt loop of Streptomyces albovinaceus AH-135Y (FERM P-12603) was inoculated to a medium (pH 7.0; 50 ml x 8) comprising glucose (20 g/L), starch (30 g/L), peptone (5 g/L), corn steep liquor (10 g/L), soybean flour (10 g/L), NaCl (3 g/L) and CaCO3 (5 g/L) and cultivated at 28degC for 48 hrs. under shaking. The inoculum was transferred to a fermentation medium and cultivated at 28degC for 96 hrs. under aeration. The cultured broth was centrifuged and the supernatant (7.2 L) was adjusted to pH 3-4. The solution was extracted with ethyl acetate and chromatographed to give (I) as a white powder (20 mg).

Member(0002)

ABEQ JP 3176672 B2 UPAB 20050509

Antiviral substance AH-135Y (I) has (1) chemical structure of formula (I); (2) elementary analysis: C 61.8%; H 5.98%, N 4.79%; (3) molecular weight of 291; (4) molecular formula of C15H17NO3; (5) m.pt. of 210-230 deg.C; (6) UV absorption spectrum (in methanol) of lamda max nm (E1%, 1 cm) of 218 (634.8), 259.5 (311.5), 342.5 (138.4); (7) IR absorption spectrum (KBr) of 3510, 1715, 1660, 1270 cm-1; (8) NMR spectrum (deuterized DMSO) of 2.29, 2.39, 2.62, 3.19, 4.51, 5.17, 7.49, 7.65, 10.77, 12.2 ppm; (9) 13C NMR spectrum (deuterized DMSO) of 20.1, 25.9, 36.9, 42.3, 57.1, 118.1, 127.2, 128.3, 130.6, 134.8, 156.2, 172.8, 205.3 ppm; (10) solubility in methanol, ethanol, acetone, ethyl acetate and dimethyl sulphoxide, and partial solubility in benzene, ether, hexane, chloroform and water ; (11) dark greenish colour reaction with alcoholic ferric chloride; (12) thin-layer chromatography; Rf 0.38 (chloroform-acetone= 3:1), 0.085 (hexane-ethyl acetate-methanol-acetic acid=10:5:0:0.5:0.1) on simical gel; and (13) white powder appearance.

Prodn. of an antiviral substance AH-135Y (I) comprises cultivating a (I)-producing microorganism of Streptomyces and recovering (I) from the cultured broth. Suitable strain can be Streptomyces albovinaceus AH-135Y (FERM P-12603).

USE - As antiviral agent. - In an example, one Pt loop of Streptomyces albovinaceus AH-135Y (FERM P-12603) was inoculated to a medium (pH 7.0; 50 ml x 8) comprising glucose (20 g/L), starch (30 g/L), peptone (5 g/L), corn steep liquor (10 g/L), soybean flour (10 g/L), NaCl (3 g/L) and CaCO3 (5 g/L) and cultivated at 28degC for 48 hrs. under shaking. The inoculum was transferred to a fermentation medium and cultivated at 28degC for 96 hrs. under aeration. The cultured broth was centrifuged and the supernatant (7.2 L) was adjusted to pH 3-4. The soln. was extracted with ethyl acetate and chromatographed to give (I) as a white powder (20 mg).

L6 ANSWER 19 OF 21 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

ACCESSION NUMBER: 1993-051545 [06] WPIDS

DOC. NO. CPI: C1993-023416 [21]

DOC. NO. NON-CPI: N1993-039245 [21]

TITLE: Determn. of water content in organic and inorganic media - by dissolving sample in heavy water and recording

NMR spectrum, at specified pH level
DERWENT CLASS: E36; J04; S03
INVENTOR: GAEVOI V A; KUTS V S
PATENT ASSIGNEE: (AUSU-R) AS UKR SURFACE CHEM INST CONS TECHN BUR
COUNTRY COUNT: 1

PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
SU 1718072	A1	19920307	(199306)*	RU	3[0]	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
SU 1718072	A1	SU 1990-4807474	19900329

PRIORITY APPLN. INFO: SU 1990-4807474 19900329
AN 1993-051545 [06] WPIDS
AB SU 1718072 A1 UPAB: 20050507
The method is based on dissolving a sample in D20 (heavy water), excitation and recording of NMR spectrum of solution and determn. of integral intensity of water protons signal. To increase the range of analysed substances to non-soluble ones and increase accuracy of determn. of water in samples containing no proton-donor gps., the samples are dissolved in D20 containing above 98% of deuterium isotope, in the ratio Po/V-D20 as 1:10 to 1:200, where Po is the weight of sample, V-D20 is volume of D20, at the time of dissolution at least 10 min., and the water content is determined by comparing the intensity of signal with that of the standard solution To increase accuracy of determn. of water content in samples containing strongly bound water, D20 is initially acidified or alkalinised to pH 5-6 or 8-9, respectively.
The solution of sample in D20 is placed in resonator of NMR -spectrometer, the spectrum is recorded and content of water in sample is determined on basis of integral intensity of signals of water protons, normalised w.r.t. internal standard (acetone or other protons-containing substance), taking correction for water content in solvent.
USE/ADVANTAGE - The method can be used in determn. of water in inorganic and organic substances and their mixts., containing no proton-donor gps. (i.e. O-H, N-H, S-H), such as salts, oxides, clays, mineral fertilisers, synthetic detergents, etc. The method extends the range of determinable substances to non-soluble ones and increases the accuracy of analysis. Bul.9/7.3.92

L6 ANSWER 20 OF 21 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 1985-186630 [31] WPIDS
DOC. NO. CPI: C1985-081373 [21]
TITLE: New antibiotic YP-0583 I-alpha - prepared by cultivating Actinoplanes microorganism in medium containing bromine cpds.
DERWENT CLASS: B04; D16
INVENTOR: IMAI Y; SOEDA Y; SUZUKI K; TAKAMURA S; WATANABE S; YAMAMOTO H
PATENT ASSIGNEE: (YAMA-C) YAMANOUCHI PHARM CO LTD
COUNTRY COUNT: 1

PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 60114194	A	19850620	(198531)*	JA	6[0]	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 60114194 A		JP 1983-223833	19831128

PRIORITY APPLN. INFO: JP 1983-223833 19831128
AN 1985-186630 [31] WPIDS
AB JP 60114194 A UPAB: 20050423
Antibiotics YP-0583 I-alpha has the following properties: (1) Appearance: white powder; (2) m.pt.: 136-137 deg.C; (3) specified UV absorption spectrum (in MeOH) IR absorption spectrum (KBr disc) and NMR spectrum (in deuterated chloroform) (4) Elemental compsn.: composed of C, H, O, Cl and Br, with one chlorine and bromine atom being contained in the molecule; (5) mol. weight (negative, fast-atom-bombardment mass spectrum method): peak observed at 1099; (6) Solubility: soluble in methanol ethanol and ethyl acetate, insoluble in water and hexane; (7) Colour reactions: FeCl3: positive (weak); 10%-H2SO4: positive; Schiff: negative; Millon:negative.
Production of antibiotic comprises growing Actinoplanes microorganism capable of producing YP-05803 I-alpha (specifically, Actinoplanes sp. YP-0583 (FERM P-7336)) in a medium containing bromine compounds. Actinoplanes sp. YP-0583 I strain is pref. grown under aerobic conditions at 18-35 deg.C and at a pH of 5 to 7.

L6 ANSWER 21 OF 21 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 1980-83216C [47] WPIDS
TITLE: Antibacterial Bu-2349A - produced by aerobic culture of microorganism of Bacillus strain in aqueous nutrient medium
DERWENT CLASS: B04; D16
INVENTOR: KAWAGUCHI H; KONISHI M; MIYAGI T; MIYAKONO T
PATENT ASSIGNEE: (BRIY-C) BRISTOL BANYU KK
COUNTRY COUNT: 1

PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 55102398	A	19800805	(198047)*	JA		
JP 01038799	B	19890816	(198936)	JA		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE

PRIORITY APPLN. INFO: US 1979-103325 19791214
US 1978-955035 19781026
US 1979-47455 19790611
AN 1980-83216C [47] WPIDS
AB JP 55102398 A UPAB: 20050419
Antibiotic Bu-234.A and its acid adduct salts are described having the properties: (i) free base form molecular formula C44H85-87N7O24-25; (ii) components: L -alanine, p-hydroxybenzoic acid, D-galactose, D-ribose, 2,4-diamino-2,4,6-trideoxyhexose, N-(8-aminobutyl)-N'-(gamma-aminopropyl)-1,4-diaminobutane, unidentified cpd. having 6 carbon atoms skelton; (iii) the antibiotic may be converted into acid adduct salts, hydrochloride salt of the substance is white amorphous solid substance; (iv) soluble in water; slightly soluble in (m)ethanol, DMSO and DMF and insoluble in organic solvent; (v) positive to ninhydrin reaction, anthron reaction, Mohrlish reaction, Fehling reagent and Remini's reagent; negative to FeCl3 and Sakaguichi's reagent; (vi) decomposes abot 215 degrees C; (vii) Anal. compsn. (Ca) C, 44.48; H 7.34; N 87; Cl 6,44, O

33.37 (%) (from difference); (viii) specific rotation (a) 2i/D = + 109 degrees (C 1.0, H2O); (ix) Gel thin layer chromatography by means of chloroform:methanol:28% ammonium hydroxide H2O (1:4:2:1 V/V) Rf 0.27; solvent methanol: 10% ammonium acetate (1:1 V/V) Rf 0.14. Solvent system-n-propanol: 28% ammonium hydroxide (4:105:60 V/V), Rf 0.06; (x) specified infrared absorption spectra (pellet in KBr) and NMR spectra (deuterium oxide 15% concentration of solution). Production of antibiotic Bu-2349A comprises aerobically culturing Bu-2349 A- producing strain of Bacillus genus in aqueous nutrient medium in immersion state.

=> d his

(FILE 'HOME' ENTERED AT 14:43:47 ON 16 JUL 2007)

FILE 'MEDLINE, BIOSIS, CAPLUS, SCISEARCH, EMBASE, WPIDS' ENTERED AT 14:46:27 ON 16 JUL 2007

L1 190 SOLUB? (S) DEUTER? (S) WATER
L2 143 DUP REM L1 (47 DUPLICATES REMOVED)
L3 41 NMR AND L2
L4 45 PY>2001 AND L2
L5 98 L2 NOT L4
L6 21 L3 AND L5

=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	121.06	122.11

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-4.68	-4.68

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=> FIL medline biosis caplus scisearch embase wpids

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FULL ESTIMATED COST	0.12	122.23

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-4.68

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FILE 'EMBASE' ENTERED AT 14:59:37 ON 16 JUL 2007

FILE 'WPIDS' ENTERED AT 14:59:37 ON 16 JUL 2007

=> solub? (s) D2O
L7 374 SOLUB? (S) D2O

=> nmr and l7
L8 107 NMR AND L7

=> py>2001 and l8
L9 32 PY>2001 AND L8

=> l8 not l9
L10 75 L8 NOT L9

=> dup rem l10
PROCESSING COMPLETED FOR L10
L11 51 DUP REM L10 (24 DUPLICATES REMOVED)

=> t ti l11 1-51

L11 ANSWER 1 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

TI Ink absorber for ink receptor used in recording sheet for ink jets, has preset spin-spin relaxation time of proton nuclear magnetic resonance spectrum, and preset restraint parameter index

L11 ANSWER 2 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
TI Novel reactivity of ruthenium alkylidenes in protic solvents: Degenerate alkylidene proton exchange

L11 ANSWER 3 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
TI Distribution and dynamics of a low-molecular-weight solute in the shell of a polymer micelle as studied by nuclear magnetic resonance

L11 ANSWER 4 OF 51 BIOSIS COPYRIGHT (c) 2007 The Thomson Corporation on STN DUPLICATE 1
TI The cooperative effect of electrostatic and hydrophobic forces in the complexation of cationic molecules by a water-soluble resorcin(4)arene derivative.

L11 ANSWER 5 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 2
TI Interface Polymerization in a Polymer Micelle: An NMR Study of the Radical Polymerization of Methyl Methacrylate at the Core-Shell Interface of Polystyrene-block-poly(methacrylic acid) Micelles

L11 ANSWER 6 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN DUPLICATE 3
TI Characterization of two structural forms of otonecine-type pyrrolizidine alkaloids from Ligularia hodgsonii by NMR spectroscopy

L11 ANSWER 7 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
TI NMR investigation on the various aggregates formed by a gemini chiral surfactant

L11 ANSWER 8 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 4
TI Fourier transform-IR and 1H NMR studies on the structure of water solubilized by reverse aggregates of calcium bis(2-ethylhexyl)

sulfosuccinate in organic solvents

L11 ANSWER 9 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
TI NMR-based amide hydrogen-deuterium exchange measurements for complex membrane proteins: Development and critical evaluation

L11 ANSWER 10 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
TI Solution structures and ligand exchange dynamics of bismuth(III) complexes with nitrilotriacetic acid and N-(2-hydroxyethyl)iminodiacetic acid

L11 ANSWER 11 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
TI Multiple deuteration of water-soluble olefinic acids with a [Pd(alizarin monosulfonate)(2)] catalyst

L11 ANSWER 12 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

TI New compound PF1195 are inhibitors of DNA synthetase and of DNA synthesis - useful as antitumour agents

L11 ANSWER 13 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

TI New glycolipids AH-2445 - are useful as antiviral agents

L11 ANSWER 14 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
TI NMR characterization and catalytic hydroformylation of water-soluble rhodium-phosphine complex in the presence of acid and base

L11 ANSWER 15 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 5
TI Study of Structure Formation in Aqueous Solutions of Poly(ethylene oxide)-Poly(propylene oxide)-Poly(ethylene oxide) Block Copolymers by Measuring Rate Constants of the Thermal Cis-Trans Isomerization of an Azobenzene Dye and Self-Diffusion of Copolymer Molecules

L11 ANSWER 16 OF 51 BIOSIS COPYRIGHT (c) 2007 The Thomson Corporation on STN DUPLICATE 6
TI Organometallic complexes with biological molecules: XII. Solid-state and solution studies on dialkyltin(IV)- and trialkyltin(IV)-thiaminepyrophosphate derivatives.

L11 ANSWER 17 OF 51 MEDLINE on STN DUPLICATE 7
TI Effect of 2'-OH acetylation on the bioactivity and conformation of 7-O-[N-(4'-fluoresceincarbonyl)-L-alanyl]taxol. A NMR -fluorescence microscopy study.

L11 ANSWER 18 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 8
TI NMR studies of the structure and interactions of block copolymer micelles in water. 4. Diffusion of organic solubilizates into the micellar core

L11 ANSWER 19 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 9
TI Noncovalent Interactions between Acenaphthenone and Dissolved Fulvic Acid As Determined by 13C NMR T1 Relaxation Measurements

L11 ANSWER 20 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 10
TI NMR study on solubility of benzyl alcohol and its transfer free energy from D2O to cationic micelle

L11 ANSWER 21 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 11
TI Use of NMR to probe the structure of water at interfaces of

organized assemblies

L11 ANSWER 22 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 12
TI Thermally Induced Structural Change of D2O-Solubilized AOT Reversed Micelles and Base-Catalyzed H-D Exchange Reaction between Solubilized D2O Deuterium and AOT-1CH Proton

L11 ANSWER 23 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 13
TI NMR and SANS Study of Poly(methyl methacrylate)-block-poly(acrylic acid) Micelles and Their Solubilization Interactions with Organic Solubilizates in D2O

L11 ANSWER 24 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 14
TI Proton NMR studies on the structure of water in ionic and nonionic water-in-oil microemulsions

L11 ANSWER 25 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
TI The preparation and characterization of some fluorinated alpha-aminoarylmethanephosphonic acids

L11 ANSWER 26 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
TI CHITOSAN-DERIVED POLYMER-SURFACTANTS AND THEIR MICELLAR PROPERTIES

L11 ANSWER 27 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 15
TI Measurement of the solubility of benzene in micellar solution by NMR

L11 ANSWER 28 OF 51 MEDLINE on STN DUPLICATE 16
TI Whole-cell detection by 13C NMR of metabolic flux through the C1-tetrahydrofolate synthase/serine hydroxymethyltransferase enzyme system and effect of antifolate exposure in Saccharomyces cerevisiae.

L11 ANSWER 29 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 17
TI 13C NMR Spin-lattice relaxation study of carbonyl carbon-water interaction in the Aerosol OT reversed micelles

L11 ANSWER 30 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 18
TI Self-Diffusion of Surfactants, Hydrocarbons, and Water in an L1 Phase and a Cubic Phase. Influence of Surfactant and Hydrocarbon Chain Lengths

L11 ANSWER 31 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
TI METAL-ASSISTED RACEMIZATION OF THE ATROPISOMERS OF A 1,1'-BINAPHTHYL SKELETON VIA A SYN TRANSITION-STATE

L11 ANSWER 32 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN
TI Solubilization in micellar solutions and phase diagram of microemulsion formation for cationic surfactant

L11 ANSWER 33 OF 51 MEDLINE on STN
TI Conformation of a water-soluble derivative of taxol in water by 2D-NMR spectroscopy.

L11 ANSWER 34 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

TI New substance WF-19849 from kernia sp. - has antifungal activity against e.g. candida albicans

L11 ANSWER 35 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN
TI Per-3,6-anhydro-α-cyclodextrin and per-3,6-anhydro-β-cyclodextrin

L11 ANSWER 36 OF 51 BIOSIS COPYRIGHT (c) 2007 The Thomson Corporation on STN DUPLICATE 19
TI SOLUBILITY OF DOMOIC ACID IN WATER AND IN NON-AQUEOUS SOLVENTS.

L11 ANSWER 37 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

TI New antibiotic TAN-390 used to treat infection and in detergent - comprises (di:sodium) epoxy:propyl-adenosine-5-di:phosphate prepared by culturing Pseudomonas

L11 ANSWER 38 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

TI New antibiotic tokimycin - obtd. by culturing streptomyces genus of actinomyces

L11 ANSWER 39 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

TI G0069C carcinostatic and antifungal cpd. production - by culturing Streptomyces strain in liquid medium in aerobic conditions

L11 ANSWER 40 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN
TI Hydrogen exchange in the hydrophilic regions of detergent-solubilized M13 coat protein detected by carbon-13 nuclear magnetic resonance isotope shifts

L11 ANSWER 41 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN
TI Mechanisms of polymer-supported catalysis. 5. Solvation of quaternary onium ions in polystyrene gels by carbon-13 NMR spectroscopy

L11 ANSWER 42 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

TI Antibiotic KA-6643-J - obtd. by fermentation using suitable streptomyces strains

L11 ANSWER 43 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN
TI A comparative study of micellar solubilization for combinations of surfactants and solubilizates using the Fourier transform pulsed-gradient spin-echo NMR multicomponent self-diffusion technique

L11 ANSWER 44 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN
TI Fourier transform NMR pulsed-gradient spin-echo (FT-PGSE) self-diffusion measurements of solubilization equilibriums in SDS solutions

L11 ANSWER 45 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

TI Antimicrobials active on plant pathogens and Gram negative bacteria - contain TAI-A as active ingredients

L11 ANSWER 46 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN
TI Binding and photoionization of N-substituted 2-chlorophenothiazines in SDS micelles

L11 ANSWER 47 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

TI (7)-Methoxy cephalosporin antibiotic Y-G 19ZD3 - prepared by culturing Streptomyces organonensis Y-G19Z

L11 ANSWER 48 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

TI (7)-Methoxy cephalosporin antibiotic Y-G 19ZD2 - prepared by culturing Streptomyces organonensis Y-G19Z

L11 ANSWER 49 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN
TI Deuterium and nitrogen-14 NMR studies of amphiphilic liquid crystals. Effect of solubilization, electrolyte and temperature on water orientation

L11 ANSWER 50 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN
TI Proton and deuteron magnetic resonance studies of lamellar lyotropic mesophases

L11 ANSWER 51 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN
TI NMR studies of the solubilization of aromatic compounds in sodium N-lauroyl sarcosinate solution

=> d ibib abs l11 1-51

L11 ANSWER 1 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 2002-064305 [09] WPIDS
DOC. NO. CPI: C2002-018785 [09]
DOC. NO. NON-CPI: N2002-047777 [09]
TITLE: Ink absorber for ink receptor used in recording sheet for ink jets, has preset spin-spin relaxation time of proton nuclear magnetic resonance spectrum, and preset restraint parameter index
DERWENT CLASS: G02; G05; P75; T04
INVENTOR: MIYAMOTO I; SATO S; SHIMIZU T
PATENT ASSIGNEE: (ASAH-C) ASAHI KASEI KOGYO KK
COUNTRY COUNT: 1

PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 2001253162	A	20010918	(200209)*	JA	8[0]	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 2001253162	A	JP 2000-66739	20000310

PRIORITY APPLN. INFO: JP 2000-66739 20000310
AN 2002-064305 [09] WPIDS
AB JP 2001253162 A UPAB: 20050524
NOVELTY - Mixture of D2O solution of acid red 18, ink absorber has spin-spin relaxation time of proton nuclear magnetic resonance spectrum (NMR) by Curr-Purr-Meiboom-Gill (CPMG) method at 30degreesC. Restraint parameter intensity obtained by performing optimization calculation of correlation of obtained magnetizing Mt, elapsed queuing time T immediately after 90degrees pulse irradiation in CPMG pulse sequence is 0.1 or more.

DETAILED DESCRIPTION - The mixture comprises 10 weight% of D2O solution of acid red 18 (water-soluble ink) and ink absorber in weight ratio of 2:1. The intensity of restraint parameter (chi) is obtained by a formula: Mt = Mo((chi)exp(-t/T2short)+(1-(chi)) exp(-t/T2long). T2 short, T2 long and (chi) are short components of spin-spin relaxation time respectively obtained by optimization calculation, long component (T2 short less than T2 long) of spin-spin relaxation time and intensity of restraint parameter (molar fraction of proton components which has T2 short in two components. INDEPENDENT CLAIMS are also included for the following:

(a) Ink receptor;

(b) Ink receptor slurry; and
(c) Recording sheet.
USE - For ink receptor used in ink receptor slurry for forming recording sheet (claimed) for ink jets.
ADVANTAGE - The printed recording sheet comprising the ink absorber has high optical intensity, excellent water resistance and light resistance.

L11 ANSWER 2 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
ACCESSION NUMBER: 2001:323714 SCISEARCH
THE GENUINE ARTICLE: 421RZ
TITLE: Novel reactivity of ruthenium alkylidenes in protic solvents: Degenerate alkylidene proton exchange
AUTHOR: Lynn D M; Grubbs R H (Reprint)
CORPORATE SOURCE: MIT, Dept Chem Engn, Cambridge, MA 02139 USA (Reprint); CALTECH, Div Chem & Chem Engn, Arnold & Mabel Beckman Labs Chem Synthesis, Pasadena, CA 91125 USA
COUNTRY OF AUTHOR: USA
SOURCE: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, (11 APR 2001) Vol. 123, No. 14, pp. 3187-3193. ISSN: 0002-7863.
PUBLISHER: AMER CHEMICAL SOC, 1155 16TH ST, NW, WASHINGTON, DC 20036 USA.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 31
ENTRY DATE: Entered STN: 27 Apr 2001
Last Updated on STN: 27 Apr 2001
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB A novel organometallic transformation is reported in which the alkylidene protons of water-soluble ruthenium alkylidenes 1 and 2 undergo nondestructive, degenerate exchange with solvent-derived deuterons in perdeuterated protic solvents such as D2O and CD3OD. Deuterated alkylidene complex (1-D) was isolated from a solution of alkylidene 1 in D2O, and the new alkylidene was fully characterized by H-1, H-2, C-13, and P-31 NMR spectroscopy and fast-atom bombardment mass spectroscopy (FAB-MS). The rate of alkylidene proton exchange for this transformation was found to correlate with the bulk dielectric constant of the solvent or solvent mixtures employed. The data support a mechanism for proton exchange involving the dissociation of a chloride ion from the ruthenium metal center. The rate of alkylidene H/D exchange for alkylidene 2 was faster than the rate of exchange for alkylidene 1, demonstrating that relative rates of exchange are influenced by the electron densities at the metal centers of these complexes. Several additional ruthenium alkylidenes were found to undergo analogous alkylidene H/D exchange reactions, including parent alkylidene (Cy3P)(2)Cl2Ru=CHPh (3) in CD2Cl2/CD3OD mixtures. These data suggest that this novel reactivity may be general for an entire class of ruthenium alkylidenes provided that protic species are available in solution and that the dielectric constant of the reaction medium is sufficiently high to ionize the halide ligands.

L11 ANSWER 3 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
ACCESSION NUMBER: 2000:937730 SCISEARCH
THE GENUINE ARTICLE: 380VM
TITLE: Distribution and dynamics of a low-molecular-weight solute in the shell of a polymer micelle as studied by nuclear magnetic resonance
AUTHOR: Kriz J (Reprint)
CORPORATE SOURCE: Acad Sci Czech Republ, Inst Macromol Chem, Heyrovsky Sq 2, CR-16206 Prague 6, Czech Republic (Reprint); Acad Sci

Czech Republ, Inst Macromol Chem, CR-16206 Prague 6, Czech Republic
COUNTRY OF AUTHOR: Czech Republic
SOURCE: LANGMUIR, (12 DEC 2000) Vol. 16, No. 25, pp. 9770-9774. ISSN: 0743-7463.
PUBLISHER: AMER CHEMICAL SOC, 1155 16TH ST, NW, WASHINGTON, DC 20036 USA.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 13
ENTRY DATE: Entered STN: 2000
Last Updated on STN: 2000

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Distribution and dynamics of methyl methacrylate (MMA) in contact with polystyrene-block-poly(methacrylic acid) micelles under the conditions of its full solubility in D2O (2 g/L) were studied by H-1 NMR methods, in particular pulsed-gradient-stimulated echo (PGSE), transverse relaxation, and rotating-frame relaxation, under varying intensity of the spin-lock field. It was found that MMA can penetrate into the micellar core after many hours at 300 K. In a freshly prepared system, MMA resides almost exclusively in the micellar shell. Its radial distribution there can be described by a Gaussian function with a maximum at the core - shell interface and a mean scatter of about 1.66 x R, where R is the radius of the core. Although it is fairly stable during the rotational and translational diffusion of the micelle as a whole, this distribution has an internal dynamics. According to the combined results of NMR, individual MMA molecules exchange their residence sites with an average correlation time of about 5 x 10(-4) s. Transient sorption of MMA molecules to methacrylic acid units is discussed as a probable explanation of this dynamics.

L11 ANSWER 4 OF 51 BIOSIS COPYRIGHT (c) 2007 The Thomson Corporation on STN DUPLICATE 1
ACCESSION NUMBER: 2001:28828 BIOSIS
DOCUMENT NUMBER: PREV200100028828
TITLE: The cooperative effect of electrostatic and hydrophobic forces in the complexation of cationic molecules by a water-soluble resorcin(4)arene derivative.
AUTHOR(S): Park, Seong Jin; Hong, Jong-In [Reprint author]
CORPORATE SOURCE: School of Chemistry and Molecular Engineering, Seoul National University, Seoul, 151-747, South Korea
SOURCE: Tetrahedron Letters, (21 October, 2000) Vol. 41, No. 43, pp. 8311-8315. print.
CODEN: TELEAY. ISSN: 0040-4039.
DOCUMENT TYPE: Article
LANGUAGE: English
ENTRY DATE: Entered STN: 10 Jan 2001
Last Updated on STN: 12 Feb 2002

AB A new water-soluble resorcin(4)arene derivative 4 was synthesized and the complexation of cationic guests in D2O was studied by 1H NMR spectroscopy. A 1:1 binding mode was elucidated by a Job's plot. The cooperative effect of electrostatic and hydrophobic interactions acts as a binding force for a strong complex formation with appropriate cationic guests in water. The thermodynamic parameters of complexation of guest I determined by a van't Hoff plot indicate that the complexation process is both enthalpically and entropically driven.

L11 ANSWER 5 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2000:137843 CAPLUS
DOCUMENT NUMBER: 132:265757
TITLE: Interface Polymerization in a Polymer Micelle: An NMR Study of the Radical Polymerization of

Methyl Methacrylate at the Core-Shell Interface of Polystyrene-block-poly(methacrylic acid) Micelles

AUTHOR(S): Kriz, J.; Kurkova, D.; Kadlec, P.; Tuzar, Z.; Plestil, J.

CORPORATE SOURCE: Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Prague, 162 06, Czech Rep.

SOURCE: Macromolecules (2000), 33(6), 1978-1985
CODEN: MAMOBX; ISSN: 0024-9297

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Systems containing poly(styrene)-block-poly(methacrylic acid) micelles (1.67 g/L), Me methacrylate (1.88-3.76 g/L), and initiator (polymerization) or inhibitor (pure solubilization) in D2O buffer solution were studied by 1H NMR. The proton NMR signals of MMA dissolved in the micellar system have the same chemical shifts as those in the corresponding D2O buffer solution but exhibit a characteristically broadened and asym. shape. Sep. signals with different chemical shifts and signal shapes were observed for MMA absorbed into the poly(styrene) core. From the shape anal. of the signals of the water-dissolved MMA in the micellar system, it can be deduced that the monomer is almost exclusively accumulated near the core-shell interface. Its radial distribution can be approximated by a Gaussian function with the maximum at the core radius R and half-width b of 1.65R and 1.93R for the MMA concns. 2 and 4 g/L, resp. An increase in temperature from 295 to 330 K leads to a faster self-diffusion of MMA but not to an appreciable broadening of the distribution. When initiated with ammonium peroxysulfate (330 K) or its mixture with potassium disulfite (295 K), MMA at the interface undergoes polymerization At elevated temps. such as 330 K, a part of MMA diffuses into the outer layers of the polystyrene core and does not polymerize there, in particular at higher MMA concns., being shielded by the peel of PMMA from the initiator radicals. At 295 K, the diffusion is very slow so that no detectable amount of MMA avoids polymerization The observed polymerization kinetics as well as the MMA signal shape evolution indicate that (i) during polymerization, the PMMA formed diffuses into the vicinity of the core-shell interface and (ii) termination is markedly suppressed in analogy with a gel effect. Math. models of the NMR signal shape as well as of diffusion-affected polymerization kinetics under general radial monomer distribution in a micelle are presented and the numerical computer simulations are compared with the exptl. data. The results of this study agree with the sep. published SANS results in the conclusion that micelles with cores sheeted with multiple layers of different polymers can be prepared by the relatively simple technique presented.

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 6 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN DUPLICATE 3

ACCESSION NUMBER: 2000:517856 SCISEARCH
THE GENUINE ARTICLE: 329TA

TITLE: Characterization of two structural forms of otonecine-type pyrrolizidine alkaloids from Ligularia hodgsonii by NMR spectroscopy

AUTHOR: Lin G (Reprint); Rose P; Chatson K B; Hawes E M; Zhao X G; Wang Z T

CORPORATE SOURCE: Chinese Univ Hong Kong, Dept Pharmacol, Special Adm Reg, Shatin, NT, Hong Kong (Reprint); Natl Res Council Canada, Inst Plant Biotechnol, Saskatoon, SK S7N 0W9, Canada; Univ Saskatchewan, Coll Pharm & Nutr, Saskatoon, SK, Canada; China Pharmaceut Univ, Dept Pharmacognosy, Nanjing, Peoples R China

COUNTRY OF AUTHOR: Hong Kong; Canada; Peoples R China
SOURCE: JOURNAL OF NATURAL PRODUCTS, (JUN 2000) Vol. 63, No. 6, pp. 857-860.
ISSN: 0163-3864.
PUBLISHER: AMER CHEMICAL SOC, 1155 16TH ST, NW, WASHINGTON, DC 20036 USA.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 22
ENTRY DATE: Entered STN: 2000
Last Updated on STN: 2000
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Clivorine (1) and ligularine (2), two hepatotoxic otonecine-type pyrrolizidine alkaloids isolated from Ligularia hodgsonii, an antitussive traditional Chinese medicine, were investigated in CDCl3 and D2O by various NMR techniques to delineate why this type of alkaloid displays uncharacteristic solubility properties by dissolving in both nonpolar organic and aqueous solutions. The results demonstrated that both alkaloids exist in a non-ionized form in CDCl3, but in an ionized form in D2O, suggesting that this unique dual solubility may play a role in the intoxication resultant from consumption of water extracts of herbs, including herbal teas,containing otonecine-type pyrrolizidine alkaloids.

L11 ANSWER 7 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
ACCESSION NUMBER: 2000:58861 SCISEARCH
THE GENUINE ARTICLE: 273GE
TITLE: NMR investigation on the various aggregates formed by a gemini chiral surfactant
AUTHOR: Luchetti L (Reprint); Mancini G
CORPORATE SOURCE: Univ Roma Tor Vergata, Dipartimento Sci & Tecnol Chim, Via Ric Sci, I-00133 Rome, Italy (Reprint); Univ Roma Tor Vergata, Dipartimento Sci & Tecnol Chim, I-00133 Rome, Italy; Univ Rome La Sapienza, Dipartimento Chim, CNR, Ctr Studio Meccanismi Reaz, I-00185 Rome, Italy
COUNTRY OF AUTHOR: Italy
SOURCE: LANGMUIR, (11 JAN 2000) Vol. 16, No. 1, pp. 161-165.
ISSN: 0743-7463.
PUBLISHER: AMER CHEMICAL SOC, 1155 16TH ST, NW, WASHINGTON, DC 20036 USA.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 16
ENTRY DATE: Entered STN: 2000
Last Updated on STN: 2000
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB In this paper we report an NMR investigation on the chiral gemini surfactant (2S,3S)-2,3-dimethoxy-1,4-bis(N-hexadecyl-N,N-dimethylammonium)butane dibromide (1), carried out to study the aggregation in various solvents. If the aggregation equilibrium of 1 can be described by the mass action law model, by observing the variation of chemical shift with respect to [1], we can obtain the aggregation number n. In CDCl3 the values are n = 2 and 19 +/- 3, at low and high [I], respectively, indicating that 1 is present in dimeric assemblies and as reversed micelles. In CD3OD, despite evidence that 1 is under aggregating conditions, the model does not hold; 1 should form a relatively flexible structure, because in the C-13 NMR spectra (1)J(C-13, N-14) coupling is observed ((1)J = 3.4 Hz). 1 is scarcely soluble in D2O; in the H-1 NMR spectrum of 1 x 10(-3) M 1, the signals relative to the tails and to one of the NCH3 groups disappear, while the other head group signals are well resolved, indicating the presence of large assemblies. These large aggregates are confirmed by

preliminary experiments of dynamic laser light scattering. The signals of the two NCH3 groups are very different in all the solvents investigated. This result can be interpreted in terms of an aggregate conformation in which they undergo different environments.

L11 ANSWER 8 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 2000:146908 CAPLUS
DOCUMENT NUMBER: 132:242259
TITLE: Fourier transform-IR and 1H NMR studies on the structure of water solubilized by reverse aggregates of calcium bis(2-ethylhexyl) sulfosuccinate in organic solvents
AUTHOR(S): Novaki, L. P.; Pires, P. A. R.; El Seoud, O. A.
CORPORATE SOURCE: Instituto de Quimica Universidade de Sao Paulo, Sao Paulo, 05599-970, Brazil
SOURCE: Colloid and Polymer Science (2000), 278(2), 143-149
CODEN: CPMSB6; ISSN: 0303-402X
PUBLISHER: Springer-Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The structure of water solubilized by reverse aggregates of calcium bis(2-ethylhexyl) sulfosuccinate in deuterobenzene and toluene has been probed by Fourier transform-IR and 1H NMR spectroscopies. The νOD band of solubilized HOD (4% D2O in H2O) has been recorded as a function of the [water]/[surfactant] molar ratio, W/S. Curve fitting of this band showed the presence of a main peak at 2550 ± 13 cm-1 and a small one at 2405 ± 15 cm-1. As a function of increasing W/S, the frequency of the main peak decreases, its full width at half-height increases, and its area increases linearly. The 1H NMR chemical shift of solubilized H2O-D2O mixts. at W/S = 18.1 has been measured as a function of the deuterium content of the aqueous nanodroplet. These data were used to calculate the so-called "fractionation factor" of the aggregate-solubilized water, the value of which was found to be unity. The results of both techniques show that reverse aggregate-solubilized water, although different from bulk water, does not seem to coexist in "layers" of different degrees of structure, as suggested, for example by the two-state water-solubilization model.
REFERENCE COUNT: 73 THERE ARE 73 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 9 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
ACCESSION NUMBER: 2000:133926 SCISEARCH
THE GENUINE ARTICLE: 282MM
TITLE: NMR-based amide hydrogen-deuterium exchange measurements for complex membrane proteins: Development and critical evaluation
AUTHOR: Czerski L; Vinogradova O; Sanders C R (Reprint)
CORPORATE SOURCE: Case Western Reserve Univ, Dept Physiol & Biophys, Cleveland, OH 44106 USA (Reprint)
COUNTRY OF AUTHOR: USA
SOURCE: JOURNAL OF MAGNETIC RESONANCE, (JAN 2000) Vol. 142, No. 1, pp. 111-119.
ISSN: 1090-7807.
PUBLISHER: ACADEMIC PRESS INC, 525 B ST, STE 1900, SAN DIEGO, CA 92101-4495 USA.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 43
ENTRY DATE: Entered STN: 2000
Last Updated on STN: 2000
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS
AB A method for measuring site-specific amide hydrogen-deuterium

exchange rates for membrane proteins in bilayers is reported and evaluated. This method represents an adaptation and extension of the approach of Dempsey and co-workers (Biophys, J. 70, 1777-1788 (1996)) and is based on reconstituting N-15-labeled membrane proteins into phospholipid bilayers, followed by lyophilization and rehydration with D2O or H2O (control), Following incubation for a time t under hydrated conditions, samples are again lyophilized and then solubilized in an organic solvent system, where H-1-N-15 HSQC spectra are recorded. Comparison of spectra from D2O-exposed samples to spectra from control samples yields the extent of the H-D exchange which occurred in the bilayers during time t. Measurements are site specific if specific N-15 labeling is used, The first part of this paper deals with the search for a suitable solvent system in which to solubilize complex membrane proteins in an amide "exchange-trapped" form for NMR quantitation of amide peak intensities. The second portion of the paper documents application of the overall procedure to measuring site-specific amide exchange rates in diacylglycerol kinase, a representative integral membrane protein. Both the potential usefulness and the significant limitations of the new method are documented. (C) 2000 Academic Press.

L11 ANSWER 10 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN

ACCESSION NUMBER: 2001:60645 SCISEARCH
THE GENUINE ARTICLE: 390LN
TITLE: Solution structures and ligand exchange dynamics of bismuth(III) complexes with nitrilotriacetic acid and N-(2-hydroxyethyl)iminodiacetic acid
AUTHOR: Asato E (Reprint); Kamamuta K; Imade R; Yamasaki M
CORPORATE SOURCE: Univ Ryukyus, Dept Chem Biol & Marine Sci, Nishihara, Okinawa 9030213, Japan (Reprint); Rigaku Corp, Xray Res Lab, Akishima, Tokyo 1968666, Japan
COUNTRY OF AUTHOR: Japan
SOURCE: INORGANIC REACTION MECHANISMS, (2000) Vol. 2, No. 1-2, pp. 57-68.
ISSN: 1028-6624.
PUBLISHER: GORDON BREACH PUBLISHING, TAYLOR & FRANCIS GROUP, 325 CHESTNUT ST, 8TH FL, PHILADELPHIA, PA 19106 USA.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 26
ENTRY DATE: Entered STN: 26 Jan 2001
Last Updated on STN: 26 Jan 2001

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The highly water-soluble bismuth complex, K-3[Bi(NTA)(2)] (1), where NTA(3-) denotes nitrilotriacetate, was prepared and characterized in the solid state by X-ray crystallography and in solution by H-1 and C-13 NMR spectroscopies. The tri-anionic species [Bi(NTA)(2)](3-) is very stable over the pH* range 4.0-9.0 (pH* - pH meter reading in D2O solution). At pH* 5.0, the ligand exchange between the bound and free NTA(3-) was investigated using the temperature-variable H-1 NMR technique to provide the activation parameters of DeltaG(298) (double dagger) = 67.8 kJ mol(-1), DeltaH(double dagger) = 48.4 kJ mol(-1) and DeltaS(double dagger) = -65.2 J K-1 mol(-1), and the rate constant of k=8.0 s(-1) at 298 K. The bismuth complexes of N-(2-hydroxyethyl)iminodiacetic acid (H(3)heida), [Bi(Hheida)](NO3) . 2H(2)O (2), [Bi(heida)H2O] . H2O (3), NH4[Bi-3(heida)(3)(OH)] . 6H(2)O . CH3OH (4), and K[Bi(Hheida)(2)] . 3H(2)O (5) were also prepared to compare their solution properties with that of the Bi-NTA solution system. Complex 5 whose structure was determined by X-ray analysis is soluble in D2O over a wide pH* range (pH* < 12) and was found to be present as the mono-anionic species [Bi(Hheida)(2)](-) over the pH* range 2.5-5.5. The ligand exchange between the bound and free Hheida(2-) at pH* 5.0 was estimated to have activation parameters of <Delta>G(298)(double dagger) =

62.9 kJ mol(-1), DeltaH(double dagger) = 28.2 kJ mol(-1), and DeltaS(double dagger) = -116.3 J K-1 mol(-1), and the rate constant of k = 59.4 s(-1) at 298 K.

L11 ANSWER 11 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN

ACCESSION NUMBER: 2000:267065 SCISEARCH
THE GENUINE ARTICLE: 300JT
TITLE: Multiple deuteration of water-soluble olefinic acids with a [Pd(alizarin monosulfonate)(2)] catalyst
AUTHOR: Papp E (Reprint); Banyai I; Joo F
CORPORATE SOURCE: Hungarian Acad Sci, Res Grp Homogeneous Catalysis, POB 7, H-4010 Debrecen, Hungary (Reprint); Hungarian Acad Sci, Res Grp Homogeneous Catalysis, H-4010 Debrecen, Hungary; Lajos Kossuth Univ, Inst Phys Chem, H-4010 Debrecen, Hungary
COUNTRY OF AUTHOR: Hungary
SOURCE: REACTION KINETICS AND CATALYSIS LETTERS, (JAN 2000) Vol. 69, No. 1, pp. 23-30.
ISSN: 0133-1736.
PUBLISHER: AKADEMIAI KIADO, PO BOX 245, H-1519 BUDAPEST, HUNGARY.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 13
ENTRY DATE: Entered STN: 2000
Last Updated on STN: 2000

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Hydrogenations in aqueous systems with the soluble [Pd(alizarin monosulfonate)(2)] catalyst resulted in extensive deuteration of crotonic, trans-2-pentenoic and itaconic acids regardless of whether the deuterium source was D-2 or D2O. Itaconic acid was deuterated up to 3.6 D/methylsuccinic acid. Detailed H-1- and C-13-NMR studies identified six isotopomers of the deuterated methylsuccinic acid product and revealed an important role of the H/D exchange on the catalytically active Pd-intermediate.

L11 ANSWER 12 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN

ACCESSION NUMBER: 2000-295670 [26] WPIDS
DOC. NO. CPI: C2000-089559 [26]
TITLE: New compound PF1195 are inhibitors of DNA synthetase and of DNA synthesis - useful as antitumour agents
DERWENT CLASS: B02; D16
INVENTOR: HOSHIKO S; IKEGAMI H; SAKUMA S; SASAKI T; TABATA Y; YAGUCHI T
PATENT ASSIGNEE: (MEIP-C) MEIJI MILK PROD CO LTD; (MEIJ-C) MEIJI SEIKA KAISHA LTD
COUNTRY COUNT: 1

PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 11269164	A	19991005	(200026)*	JA	6[0]	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 11269164 A		JP 1998-90593	19980320

PRIORITY APPLN. INFO: JP 1998-90593 19980320
AN 2000-295670 [26] WPIDS
AB JP 11269164 A UPAB: 20050410

NOVELTY - Compound PF1195 (I) and its salts are new. DETAILED DESCRIPTION - Compound PF1195 of formula (I) and its salts are new. (I) have the following physicochemical properties: (1) colour and appearance: yellow powder; (2) m.pt.: decomposes at 190 °C without showing definite m.pt.; (3) mass spectrometry: FAB-MS (m/z) 825 [M+H]+, HRFAB-MS (m/z) calculated. 825.1668, found 825.16661 [M+H]+, (4) specific rotation: [α]D = -371 °(c 0.5, MeOH); (5) UV absorption spectrum in MeOH solution: λnm (epsilon) 218 (50500), 269 (29600), 325 (35000); (6) IR absorption spectrum (KBr) 3400, 1720, 1624, 1595, 1543, 1450; (7) 1H-NMR spectrum data determined in D2O; (8) 13C-NMR spectrum data determined in heavy DMSO; and (9) solubility: soluble in DMSO and MeOH. An INDEPENDENT CLAIM is included for the preparation of (I) using a culture of PF1195-producing Talaromyces sp. microorganism.

USE - (I) are inhibitors of DNA synthetase and of DNA synthesis. (I) are useful as antitumour agents.

L11 ANSWER 13 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 1999-544952 [46] WPIDS
DOC. NO. CPI: C1999-159363 [46]
TITLE: New glycolipids AH-2445 - are useful as antiviral agents
DERWENT CLASS: B04; D16
INVENTOR: UEDA M; YOKOMIZO K
PATENT ASSIGNEE: (KAGA-C) ZH KAGAKU & KESSEI RYOHO KENKYUSHO
COUNTRY COUNT: 1

PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 11236393	A	19990831	(199946)*	JA	13[8]	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 11236393 A		JP 1998-323542	19981113

PRIORITY APPLN. INFO: JP 1997-337983 19971120
AN 1999-544952 [46] WPIDS
AB JP 11236393 A UPAB: 20050523
Antiviral glycolipids AH-2445 of formula (I) are new: n, n', n'', n''' = number of side chain methylene group(s), provided N = n+n'+n''+n''' = 32-56, particularly N = 45; and n = 14; n', n'' = 13; and n''' = 5.

USE - As antiviral agents.

L11 ANSWER 14 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
ACCESSION NUMBER: 1999:771962 SCISEARCH
THE GENUINE ARTICLE: 245YV
TITLE: NMR characterization and catalytic hydroformylation of water-soluble rhodium-phosphine complex in the presence of acid and base
AUTHOR: Zhang Y; Yuan Y Z (Reprint); Liao X L; Ye J L; Yao C X; Tsai K
CORPORATE SOURCE: Xiamen Univ, Dept Chem, Inst Phys Chem, State Key Lab Phys Chem Solid Surface, Xiamen 361005, Peoples R China (Reprint)
COUNTRY OF AUTHOR: Peoples R China
SOURCE: CHEMICAL JOURNAL OF CHINESE UNIVERSITIES-CHINESE, (OCT 1999) Vol. 20, No. 10, pp. 1589-1594.
ISSN: 0251-0790.
PUBLISHER: HIGHER EDUCATION PRESS, SHATANHOU ST 55, BEIJING 100009,

PEOPLES R CHINA.
DOCUMENT TYPE: Article; Journal
LANGUAGE: Chinese
REFERENCE COUNT: 14
ENTRY DATE: Entered STN: 1999
Last Updated on STN: 1999
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB When NaOH was added into D2O-soiution of HRh(CO)(TPPTS)(3)[TPPTS: P(m-C6H4SO3Na)(3), trisodium salt of tri-(m-sulfophenyl)-phosphine], there were no changes in the characteristic peaks for the water-soluble complex although a small peak at delta 35.1 for OTPPTS[OTPPTS: O = P(m-C6H4SO3Na)(3), trisodium salt of tri-(nz-sulfophenyl)-phosphine oxide] was formed under a high concentration of NaOH, as evidenced by the spectra of P-31(H-1) NMR and H-1 NMR, indicating that the influence on the molecular structure of the complex by NaOH may be limited. Several new signals at delta 29-34 accompanied by the appearance of free ligand TPPTS at delta - 5.0- - 5.3 appeared in the P-31(IH) NMR spectra when pyridine was introduced into HRh(CO)(TPPTS)(3), probably due to the reaction of ligand exchange among the coordinated ligands(such as TPPTS, hydrogen, and CO) in the complex HRh(CO) (TPPTS)(3) and pyridine molecule. The water-soluble complex can be readily decomposed, however, when inorganic acids such as HCl, H2SO4, HNO3 and H3PO4 were introduced into the D2O-solution of HRh(CO)(TPPTS)(3), as shown in P-31(H-1) NMR spectroscopic data. The decomposition of the complex was completed by the formation of OTPPTS at delta 35. 1 and some new phosphate species at delta 27-29 in the P-31(H-1) NMR spectra in the presence of above inorganic acids. Analogous results to those by addition of inorganic acid were obtained when acetate acid was exceeded in mole ratio to HRh(CO)(TPPTS)(3). An increment in n/i ratio of heptyl aldehydes and a depression in TOF were obtained in case of the addition of base, in contrary, a lower n/i ratio of aldehydes in yellowish product was obtained in case of the addition of acid in I-hexene hydroformylation catalyzed by HRh (CO)(TPPTS)(3). The results obtained showed that the molecular structure and catalytic performance of HRh (CO)(TPPTS)(3) may be affected by acid more disserviceably than by base.

L11 ANSWER 15 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 1999:49878 CAPLUS
DOCUMENT NUMBER: 130:197267
TITLE: Study of Structure Formation in Aqueous Solutions of Poly(ethylene oxide)-Poly(propylene oxide)-Poly(ethylene oxide) Block Copolymers by Measuring Rate Constants of the Thermal Cis-Trans Isomerization of an Azobenzene Dye and Self-Diffusion of Copolymer Molecules
AUTHOR(S): Gille, Kathrin; Knoll, Helmut; Rittig, Frank; Fleischer, Gerald; Kaerger, Joerg
CORPORATE SOURCE: Wilhelm-Ostwald-Institut fuer Physikalische und Theoretische Chemie, Fakultaet fuer Chemie und Mineralogie der Universitaet Leipzig, Leipzig, D-04103, Germany
SOURCE: Langmuir (1999), 15(4), 1059-1066
CODEN: LANGD5; ISSN: 0743-7463
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In aqueous solns. of poly(ethylene oxide) (PEO)-poly(propylene oxide) (PPO)-PEO triblock copolymers (Pluronics P85, F88, and L64), structure formation (micellization) on increasing temperature was followed by determination of rate consts. kiso of the thermal cis-trans isomerization of 4,4'-nitroanilinoazobenzene by means of flash photolysis in H2O and D2O.

The kinetic solvent isotope effect kiso,H2O/kiso,D2O indicates that the azobenzene dye mols. are solubilized in a water-rich environment. From the nearly constant solvatochromic UV/vis absorption band maxima λmax of the dye, it is concluded that the S shape of the ln kiso vs 1/T curves is mainly due to microviscosity changes on micellization. Critical micelle temperature values derived are in satisfactory agreement with those from self-diffusion coeffs. of the copolymer mols. dependent on temperature determined by means of pulsed field gradient NMR measurements. The self-diffusion expts. allow conclusions on the size of the diffusing particles in H2O and D2O and the influence of dye mols. on aggregation. The hydrodynamic radii of the diffusing species are larger in H2O than in D2O. The reason is seen in the stronger hydrogen bonds between EO units and D2O compared to those between EO units and H2O. On gelation of 25% (w/v) F88 in water at 31° C, the bulk viscosity increases sharply but the microviscosity around the dye mols. does not.

REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 16 OF 51 BIOSIS COPYRIGHT (c) 2007 The Thomson Corporation on STN DUPLICATE 6

ACCESSION NUMBER: 2000:736 BIOSIS
DOCUMENT NUMBER: PREV200000000736
TITLE: Organometallic complexes with biological molecules: XII. Solid-state and solution studies on dialkyltin(IV)- and trialkyltin(IV)-thiaminepyrophosphate derivatives.
AUTHOR(S): Fiore, T.; Pellerito, C.; Fontana, A.; Triolo, F.; Maggio, F.; Pellerito, L. [Reprint author]; Cestelli, A.; Di Liegro, I.
CORPORATE SOURCE: Dipartimento di Chimica Inorganica, Universita di Palermo, Viale delle Scienze, Parco D'Orleans, 90128, Palermo, Italy
SOURCE: Applied Organometallic Chemistry, (Oct., 1999) Vol. 13, No. 10, pp. 705-714. print.
CODEN: AOCHEX. ISSN: 0268-2605.
DOCUMENT TYPE: Article
LANGUAGE: English
ENTRY DATE: Entered STN: 23 Dec 1999
Last Updated on STN: 31 Dec 2001

AB Dialkyltin(IV) and trialkyltin(IV) derivatives of the coenzyme thiaminepyrophosphate (H2TPP) have been synthesized with general formula R2Sn(HTPP)2cntdotnH2O (Alk = Me, n = 2; Alk = Bu, n = 4) and R3SnHTPPcntdotnH2O (R=Me, n = 2; R = Bu, n = 1), respectively. The solid-state structure of the complexes has been investigated through infrared and Mossbauer spectroscopy. The infrared data suggest the involvement of only phosphate oxygen atoms in the coordination of both dialkyl- and trialkyl-tin(IV) moieties, with phosphate anions behaving as monoanionic bidentate bridging or chelating groups, with the tin(IV) involved in six- and five-fold coordination geometries, respectively, in R2Sn(HTPP)2cntdotnH2O (R = Me, n = 2; R = Bu, n = 4) and R3SnHTPPcntdotnH2O (R = Me, n = 2; R = Bu, n = 1). The 119Sn Mossbauer data, and in particular rationalization of the experimental nuclear quadrupole splittings, DELTA, through the point-charge model formalism, suggests the occurrence of an octahedral trans-R2 structure in R2Sn(HTPP)2cntdotnH2O (R = Me, n = 2; R = Bu, n = 4) and a trigonal-bipyramidal structure in R3SnHTPPcntdotnH2O (R = Me, n = 2; R = Bu, n = 1). 1H and 13C NMR spectra, in D2O, suggested that the soluble derivatives, at room temperature, in solution, maintained the solid-state structure. The interactions of dibutyltin(IV)-thiaminepyrophosphate (DBTPP) and tributyltin(IV)-thiaminepyrophosphate (TBTPP) complexes with Bluescript KS(+) plasmid and immortalized 3T3 fibroblasts were studied. Both compounds have a clear inhibitory effect on the growth of immortalized mouse embryonal fibroblasts (NIH-3T3), TBTPP being the much more active. No evidence was found, however, for DNA cleavage by the compounds at molar ratios as high

as 1:10 (DBTPP, TBTPP/DNA base pairs). According to our observations, the cytotoxicity of TBTPP does not seem to be based on direct interaction with DNA, but in the presence of TBTPP (1:10, TBTPP/DNA bp), plasmid DNA seems to be more susceptible to cleavag e by UV.

L11 ANSWER 17 OF 51 MEDLINE on STN DUPLICATE 7
ACCESSION NUMBER: 1999056394 MEDLINE
DOCUMENT NUMBER: PubMed ID: 9839015
TITLE: Effect of 2'-OH acetylation on the bioactivity and conformation of 7-O-[N-(4'-fluoresceincarbonyl)-L-alanyl]taxol. A NMR-fluorescence microscopy study.
AUTHOR: Jimenez-Barbero J; Souto A A; Abal M; Barasoain I; Evangelio J A; Acuna A U; Andreu J M; Amat-Guerri F
CORPORATE SOURCE: Instituto de Quimica Organica, CSIC, Madrid, Spain.
SOURCE: Bioorganic & medicinal chemistry, (1998 Oct) Vol. 6, No. 10, pp. 1857-63.
Journal code: 9413298. ISSN: 0968-0896.
PUB. COUNTRY: ENGLAND: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
(RESEARCH SUPPORT, NON-U.S. GOV'T)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199901
ENTRY DATE: Entered STN: 9 Feb 1999
Last Updated on STN: 9 Feb 1999
Entered Medline: 22 Jan 1999

AB The relationship between conformation, 2'-OH acetylation, and bioactivity of two fluorescent taxoids has been investigated by a combination of NMR and fluorescence microscopy techniques. These taxoids present the structure of taxol with the 7-OH group esterified with the N-(4'-fluoresceincarbonyl)-L-alanine group and with the 2'-OH group free (taxoid 2) or acetylated (taxoid 3). The larger water solubility of 2 and 3 compared with taxol allowed a detailed NMR study in DMSO-d6/D2O (3/7), showing that both taxoids adopt a similar collapsed conformation in which the hydrophobic groups 2-O-benzoyl, 3'-phenyl and 4-O-acetyl are in close proximity, with the fluorescein group displaying unrestricted motion. On the other hand, while taxoid 2 retains essentially the ability of taxol to induce in vitro microtubule assembly and to bind to cell microtubules, the 2'-acetylated derivative 3 does not show immediate activity. However, when taxoid 3 is left in the cell culture, the slow hydrolysis of the 2'-acetate group in the medium liberates the cytotoxic, microtubule-specific taxoid 2. The intense emission of this active derivative (2) allows the accurate recording of the drug-cell interaction from the very initial steps using fluorescence microscopy. These experiments show conclusively, for the first time in cell cultures, that a free 2'-OH group in taxol is essential for the recognition of the drug by the binding site of cellular microtubules.

L11 ANSWER 18 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 8
ACCESSION NUMBER: 1997:429547 CAPLUS
DOCUMENT NUMBER: 127:51315
TITLE: NMR studies of the structure and interactions of block copolymer micelles in water. 4. Diffusion of organic solubilizates into the micellar core
AUTHOR(S): Kriz, J.; Masar, B.; Doskocilova, D.
CORPORATE SOURCE: Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Prague, 162 06, Czech Rep.
SOURCE: Macromolecules (1997), 30(15), 4391-4397
CODEN: MAMOBX; ISSN: 0024-9297
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal
LANGUAGE: English
AB Solubilization of relatively hydrophobic organic compds. (solubilizates) by the core of poly(Me methacrylate)-block-poly(acrylic acid) (PMMA-PAAc) micelles in D2O was theor. simulated and exptl. studied for chloroform, chlorobenzene, 4-methylcyclohexanone, benzene, toluene, cyclohexane, and hexane. The exptl. results show that (a) the core-captured amount of the solubilizate as well as its solubilization rate chiefly depend on its interaction with PMMA (expressed, e.g., by its χ-parameter), (b) the limiting solubilization degree may also be determined by other thermodn. factors, in particular the core-water interphase tension, (c) the solubilization rate and partly the equilibrium solubilization degree are also influenced by shell-core interactions, (d) most solubilizates, except chloroform, swell the core with a surprisingly narrow front, which could indicate a steep concentration dependence of their diffusion coefficient but also (e) there is morphol. inhomogeneity of the core with more easily accessible domains in the outer part of the core. The last conclusion is also supported by the much lower solubilization rates observed with micelles formed by copolymers with longer PMMA blocks.

L11 ANSWER 19 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 9
ACCESSION NUMBER: 1997:44384 CAPLUS
DOCUMENT NUMBER: 126:50755
TITLE: Noncovalent Interactions between Acenaphthenone and Dissolved Fulvic Acid As Determined by 13C NMR T1 Relaxation Measurements
AUTHOR(S): Nanny, Mark A.; Bortiatynski, Jacqueline M.; Hatcher, Patrick G.
CORPORATE SOURCE: Fuel Science Program, Pennsylvania State University, University Park, PA, 16802, USA
SOURCE: Environmental Science and Technology (1997), 31(2), 530-534
CODEN: ESTHAG; ISSN: 0013-936X
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Non-covalent interactions between 13C-labeled acenaphthenone (13C-labeled in the carbonyl position) and Suwannee River fulvic acid in a methanol/D2O solvent have been examined using 13C NMR T1 relaxation measurements. The influence of solvents upon the non-covalent interactions were assessed by examining acenaphthenone in pure solvents of varying solvation capacity (chloroform, methanol, methanol/D2O). Interactions with fulvic acid were examined as a function of acenaphthenone and fulvic acid concns., fulvic acid counter-cation (H+ or Na+), and pH. In the presence of fulvic acid in a methanol/D2O solvent, three non-covalent interactions were identified: a weak sorption interaction between acenaphthenone and fulvic acid, an enhanced solubilization of acenaphthenone by fulvic acid, and an interaction between just the solvent and acenaphthenone. The enhanced solubilization is hypothesized to arise from fulvic acid forming hydrophobic regions that are predominantly solvated with methanol and have excluded water. Acenaphthenone in these hydrophobic regions displays similar behavior to when it is dissolved in pure methanol. The ability of fulvic acid to form hydrophobic regions was found to be dependent upon the identity of the fulvic acid counter-cation and upon pH.
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 20 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 10
ACCESSION NUMBER: 1998:30416 CAPLUS
DOCUMENT NUMBER: 128:172429

TITLE: NMR study on solubility of benzyl alcohol and its transfer free energy from D2O to cationic micelle
AUTHOR(S): Shen, Qiang; Li, Gan-Zuo; Ma, Cheng-Song; Hao, Shu-Xuan; Wei, Xi-Lian; Huang, Yan-Zhang
CORPORATE SOURCE: Key Laboratory for Colloid and Interface Chemistry of State Education Commission, Shandong University, Jinan, 250100, Peop. Rep. China
SOURCE: Chinese Journal of Chemistry (1997), 15(5), 405-409
CODEN: CJOCEV; ISSN: 1001-604X
PUBLISHER: Science Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new kind of surfactant, [CnH2n+1OCH2CH(OH)CH2N(CH3)3]Cl (n=12, 14, 16) was synthesized. The solubility of benzyl alc. in micellar solns. was determined by 1H NMR method. The results indicate that the length of alkyl chains of the surfactant affects the solubility of benzyl alc. in 2.5+10-2 mol/L micellar solns. The solubility of benzyl alc. per L of micellar solution is 0.095 mol for n=12, 0.115 mol for n=14, 0.165 mol for n=16. The transfer free energy of benzyl alc. from aqueous phase to micellar phase is -24.29 kJ/mol for n=12, -24.37 kJ/mol for n=14, -24.49 kJ/mol for n=16.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 21 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 11
ACCESSION NUMBER: 1997:456500 CAPLUS
DOCUMENT NUMBER: 127:210588
TITLE: Use of NMR to probe the structure of water at interfaces of organized assemblies
AUTHOR(S): El Seoud, Omar A.
CORPORATE SOURCE: Instituto de Quimica, Universidade de Sao Paulo, C.P. 26.077, Sao Paulo, S.P., 05599-970, Brazil
SOURCE: Journal of Molecular Liquids (1997), 72(1/3), 85-103
CODEN: JMLIDT; ISSN: 0167-7322
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review with 58 refs. which addresses the use of NMR spectroscopy to probe the structure of interfacial water of organized assemblies: aqueous micelles, reverse micelles, RMs, and water-in-oil microemulsions, W/O μEs. For aqueous micelles, the dependence of the 1H NMR chemical shift of water on [surfactant] is measured in H2O-D2O mixts. In case of RMs and W/O μEs, one dets. the dependence of 1H NMR chemical shift of solubilized H2O-D2O, and/or 1H and 13C chemical shifts of the surfactant headgroup on the deuterium content of solubilized water. The measured deuterium isotope effect on the appropriate chemical shift is then used to calculate the so called "deuterium/protium fractionation factor, .vphi." for interfacial water. Values of .vphi. thus obtained are rationalized in terms of effects of the interface on the structure of its water of hydration, relative to that of bulk water. The important conclusions of this review are: (1) effects of simple ions (e.g., butylsulfate or butyltrimethylammonium) on the structure of water are different from those of micellized ions (e.g., dodecylsulfate or cetyltrimethylammonium plus the associated counterions), this difference is due to electrostriction of water by the charged interface; (2) perturbation of the structure of interfacial water is larger for ionic micelles than for the corresponding zwitterionic ones; (3) For the same class of surfactants, e.g., cationic or zwitterionic, the micelle-induced enhancement of the structure of interfacial water (relative to that of bulk water) increases as a function of increasing the

hydrophobic character of the surfactant headgroup; (4) Water solubilized by RMs and W/O μEs does not seem to coexist in "layers" of different structures within the micellar water "pool".

REFERENCE COUNT: 103 THERE ARE 103 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 22 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 12
ACCESSION NUMBER: 1996:256523 CAPLUS
DOCUMENT NUMBER: 124:299570
TITLE: Thermally Induced Structural Change of D2O-Solubilized AOT Reversed Micelles and Base-Catalyzed H-D Exchange Reaction between Solubilized D2O Deuterium and AOT-1CH Proton
AUTHOR(S): Yoshino, Akihiro; Okabayashi, Hirofumi; Uchida, Toshihisa; Ogasawara, Toshiaki; Yoshida, Tadayoshi; O'Connor, Charmian J.
CORPORATE SOURCE: Department of Applied Chemistry, Nagoya Institute of Technology, Nagoya, 466, Japan
SOURCE: Journal of Physical Chemistry (1996), 100(20), 8418-24
CODEN: JPCHAX; ISSN: 0022-3654
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The temperature dependence of the 1H NMR spectrum for the D2O -solubilized Aerosol-OT (AOT)-C6D6 system in the reversed micellar state was studied at 323-353 K. From the 1H chemical shift variation of the AOT polar segment protons and of the HDO proton, a structural transition of H2O incorporated into the polar core occurs at 343 K and this transition is the result of the variation in interaction between H2O mols. within the polar core and those solubilized at or close to polar head groups of the ethylhexyl chains. The base-catalyzed H-D exchange reaction between the AOT-1CH proton and solubilized D2O D was studied in this temperature range. Kinetic anal. (based on the time dependence of the 1H NMR spectrum) allowed evaluation of the thermodn. parameters of the exchange reaction. These show a marked difference between the 2 temperature ranges 323-343 and 343-353 K. In particular, the 13C chemical shift data indicate that the local concentration of the OD- anions has a considerable influence on the H-D exchange reaction at 323-353 K.

L11 ANSWER 23 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 13
ACCESSION NUMBER: 1996:644016 CAPLUS
DOCUMENT NUMBER: 125:330053
TITLE: NMR and SANS Study of Poly(methyl methacrylate)-block-poly(acrylic acid) Micelles and Their Solubilization Interactions with Organic Solubilizates in D2O
AUTHOR(S): Kriz, J.; Masar, B.; Pospisil, H.; Plestil, J.; Tuzar, Z.; Kiselev, M. A.
CORPORATE SOURCE: Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Prague, 162 02, Russia
SOURCE: Macromolecules (1996), 29(24), 7853-7858
CODEN: MAMOBX; ISSN: 0024-9297
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Poly(Me methacrylate)-block-poly(acrylic acid) copolymers (PMMA-PAAc) neutralized to various degrees with Li, Na, or K counterions were synthesized and their micellar solns. in D2O were studied using 1H and 7Li NMR and SANS. The micelles solubilize organic substances such as

chloroform or chlorobenzene under swelling of their PMMA cores with a kinetics controlled mainly by the interaction parameter between the solubilizate and PMMA. The solubilizate is shown to be mainly distributed in the inner area of the micellar corona in the early stages of the solubilization process, later both in the micellar core and along the chains of the corona, in particular in the case of PMMA-PAAc micelles in their acid form. By neutralizing the PAAc chains to various degrees and observing both the NMR spectra and the longitudinal relaxation rate of 1H and 7Li, changes of conformation and mobility of the PAAc chains can be deduced. With increasing neutralization degree, the solubilization is accelerated but the equilibrium degree of solubilization is slightly lower. The solubilizate transport between PMMA-PAAc and polystyrene-block-poly(methacrylic acid) (PS-PMAc) in their sodium forms is demonstrated by showing the solubilization selectivity.

L11 ANSWER 24 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 14
ACCESSION NUMBER: 1996:528998 CAPLUS
DOCUMENT NUMBER: 125:178074
TITLE: Proton NMR studies on the structure of water in ionic and nonionic water-in-oil microemulsions
AUTHOR(S): El Seoud, Omar A.; Okano, Laura T.; Novaki, Luzia P.; Barlow, Graham K.
CORPORATE SOURCE: Inst. Quimica, Univ. Sao Paulo, Sao Paulo, 05599-970, Brazil
SOURCE: Berichte der Bunsen-Gesellschaft (1996), 100(7), 1147-1152
CODEN: BBPCAX; ISSN: 0940-483X
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The structure of H2O present in water-in-oil microemulsions of anionic Mg bis(2-ethylhexyl) sulfosuccinate in C6D6, cationic cetyldimethylbenzylammonium chloride in C6D6, cetyldimethyl-3-phenylpropylammonium chloride in chlorobenzene, and nonionic polyoxyethylene (4) dodecyl ether (Brij 30, C12E4) in heptane was probed by 1H NMR. Chemical shifts of solubilized water-D2O, and of surfactant discrete protons were determined (at fixed [water]/[surfactant] ratios) as a function of the D content of solubilized H2O. Chemical shift data were used to calculate the so-called "fractionation factor" (ϕ) of the aggregate-solubilized H2O. The calculated ϕ for the different systems are 1, showing that micellar H2O (although different from bulk H2O) does not seem to coexist in "layers" of different degrees of structure, as suggested, e.g., by the 2-state H2O solubilization model.

L11 ANSWER 25 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
ACCESSION NUMBER: 1996:702300 SCISEARCH
THE GENUINE ARTICLE: VH779
TITLE: The preparation and characterization of some fluorinated alpha-aminoarylmethanephosphonic acids
AUTHOR: Green D S C (Reprint); Gruss U; Hagele G; Hudson H R; Lindblom L; Pianka M
CORPORATE SOURCE: UNIV DUSSELDORF, INST ANORGAN CHEM & STRUKTURCHEM 1, D-40225 DUSSELDORF, GERMANY; UNIV N LONDON, SCH APPL CHEM, LONDON N7 8DB, ENGLAND
COUNTRY OF AUTHOR: GERMANY; ENGLAND
SOURCE: PHOSPHORUS SULFUR AND SILICON AND THE RELATED ELEMENTS, (1996) Vol. 113, No. 1-4, pp. 179-207.
ISSN: 0308-664X.
PUBLISHER: GORDON BREACH SCI PUBL LTD, C/O STBS LTD PO BOX 90, READING, BERKS, ENGLAND RG1 8JL.
DOCUMENT TYPE: Article; Journal

FILE SEGMENT: PHYS
LANGUAGE: English
REFERENCE COUNT: 56
ENTRY DATE: Entered STN: 1996
Last Updated on STN: 1996
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB alpha-Aminoarylmethanephosphonic acids have been prepared with a range of fluoro, fluoroalkyl, or fluoroalkoxy substituents in the benzene ring (4-F, 3-F, 2-F, 3,4-F-2, F-5, 4-CF3, 3-CF3, 4-CF3O, and 3-CF3O). These compounds have relatively low aqueous solubility and their NMR spectra (H-1, C-13, P-31 and F-19) were therefore recorded in D2O in the presence of an excess of alkali. Under these conditions, the ring substituents appear to have Little effect on delta(p)(15-18 ppm), or on the H-1 and C-13 parameters for the benzylic group (alpha-CH), which are mainly in the ranges observed for other types of alpha-aminoarylmethanephosphonic acids under alkaline conditions (delta(H) 3.8-4.0 ppm, (2)J(PH) 15.3-16.5 Hz; delta(C) 57-58 ppm, (1)J(PC) 128-132 Hz). For those examples with fluorine in the ortho position (i.e., the 2-fluoro and pentafluoro derivatives) a slightly higher field chemical shift was observed for the benzylic carbon atom (delta(C), 50-51 ppm). In the fast-atom bombardment mass spectra, pseudo-molecular ions, MH(+), and ions resulting from the elimination of phosphorous acid [MH-H3PO3](+), provide a further useful means of characterization for these compounds.

L11 ANSWER 26 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN
ACCESSION NUMBER: 1995:750335 SCISEARCH
THE GENUINE ARTICLE: TC412
TITLE: CHITOSAN-DERIVED POLYMER-SURFACTANTS AND THEIR MICELLAR PROPERTIES
AUTHOR: YOSHIOKA H (Reprint); NONAKA K; FUKUDA K; KAZAMA S
CORPORATE SOURCE: SHIZUOKA UNIV, GRAD SCH NUTR & ENVIRONM SCI, 52-1 YADA, SHIZUOKA 422, JAPAN (Reprint); SHIZUOKA UNIV, SCH PHARMACEUT SCI, SHIZUOKA 422, JAPAN
COUNTRY OF AUTHOR: JAPAN
SOURCE: BIOSCIENCE BIOTECHNOLOGY AND BIOCHEMISTRY, (OCT 1995) Vol. 59, No. 10, pp. 1901-1904.
ISSN: 0916-8451.
PUBLISHER: JAPAN SOC BIOSCI BIOTECHN AGROCHEM, JAPAN ACAD SOC CTR BLDG, 2-4-6 YAYOI BUNKYO-KU, TOKYO, 113, JAPAN.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 14
ENTRY DATE: Entered STN: 1995
Last Updated on STN: 1995
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Chitosan derivatives, sulfated N-acyl-chitosan (S-C-n-chitosan) possessing various lengths of alkyl chain, were prepared, and the properties of their aqueous solutions were examined, The H-1-NMR spectrum of D2O solutions of S-C-12-chitosan showed broadening of the proton signals caused by aggregation of the alkyl chain, The solubility of a hydrophobic compounds, azobenzene, was small in the aqueous solutions of S-C-n-chitosan with shorter alkyl chains, but increased with increasing length of the chains above C-10, showing that micelles had been formed.

The ESR spectrum of a spin probe, TEMPO, in an S-C-14-chitosan solution showed the existence of a hydrophobic region in the solution, but this region did not exist in the S-C-2-chitosan solution, The rigidity of this region was examined by using a spin probe, 16-doxyl-stearic acid, From these results, it was revealed that S-C-n-chitosan with longer alkyl chains formed a novel type of micelle called a ''polymer micelle,'' which was more stable than the ordinary micelles formed from

low-molecular-weight surfactants.

L11 ANSWER 27 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 15
ACCESSION NUMBER: 1995:697433 CAPLUS
DOCUMENT NUMBER: 123:297311
TITLE: Measurement of the solubility of benzene in micellar solution by NMR
AUTHOR(S): Duns, G. J.; Reeves, L. W.; Yang, D. W.; Williams, D. S.
CORPORATE SOURCE: Dep. Chem., Univ. Waterloo, Waterloo, ON, N2L 3G1, Can.
SOURCE: Journal of Colloid and Interface Science (1995), 173(2), 261-4
CODEN: JCISA5; ISSN: 0021-9797
PUBLISHER: Academic
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The solubilities of benzene in micellar solns. of cetyltrimethylammonium bromide (CTAB)/D2O and decyltrimethylammonium bromide (DTAB)/D2O, and in D2O have been determined by 1H NMR spectroscopy. The average solubility of benzene in 0.15 M CTAB/D2O was found to be 3.35 ± 0.05% (wt/wt) (benzene/0.15 M CTAB/D2O), 1.18 ± 0.09% (wt/wt) (benzene/0.15 MDTAB/D2O) in 0.15 M DTAB/D2O, and 0.074 ± 0.004% (wt/wt) (benzene/D2O) in D2O. Values of ΔG = -5.0 kcal/mol and -4.8 kcal/mol were determined for the free energy of transfer of benzene from D2O to micelle for 0.15 M CTAB/D2O and 0.15 M DTAB/D2O micellar solns., resp.

L11 ANSWER 28 OF 51 MEDLINE on STN DUPLICATE 16
ACCESSION NUMBER: 94271770 MEDLINE
DOCUMENT NUMBER: PubMed ID: 8003483
TITLE: Whole-cell detection by 13C NMR of metabolic flux through the C1-tetrahydrofolate synthase/serine hydroxymethyltransferase enzyme system and effect of antifolate exposure in Saccharomyces cerevisiae.
AUTHOR: Pasternack L B; Laude D A Jr; Appling D R
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Texas, Austin 78712.
SOURCE: Biochemistry, (1994 Jun 14) Vol. 33, No. 23, pp. 7166-73.
Journal code: 0370623. ISSN: 0006-2960.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
(RESEARCH SUPPORT, NON-U.S. GOV'T)
(RESEARCH SUPPORT, U.S. GOV'T, NON-P.H.S.)
(RESEARCH SUPPORT, U.S. GOV'T, P.H.S.)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199407
ENTRY DATE: Entered STN: 29 Jul 1994
Last Updated on STN: 6 Feb 1998
Entered Medline: 21 Jul 1994
AB Folate-mediated one-carbon metabolism is critical for the synthesis of numerous cellular constituents required for cell growth. A potential source of one-carbon units is formate. This one-carbon unit is activated to 10-formyltetrahydrofolate via the synthetase activity of the trifunctional enzyme C1-tetrahydrofolate (THF) synthase for use in purine synthesis or can be further reduced to 5,10-methylene-THF by the dehydrogenase activity of the same enzyme. 5,10-Methylene-THF is used by serine hydroxymethyltransferase (SHMT) in the synthesis of serine. Recently, 13C NMR has been used to establish that the C1-THF synthase/SHMT enzyme system is the only route from formate to serine in vivo in the yeast Saccharomyces cerevisiae [Pasternack et al. (1992) Biochemistry 31, 8713-8719]. In vitro studies have considered the

kinetics of the C1-THF synthase/SHMT enzyme system in the catalytic conversion of formate to serine [Strong et al. (1987) J. Biol. Chemical 262, 12519-12525]. In the present work, we begin to study the kinetics of this two-enzyme system in its natural environment. Provision of [13C]formate and direct detection of an intracellular accumulating pool of [3-13C]serine by 13C NMR of whole cells allow us to monitor the rate of flux through this enzyme system in vivo. The rate of accumulation of soluble [3-13C]serine under [13C]formate-saturating conditions is 13.0 +/- 1.2 microM/min relative to an external standard of serine in D2O. The extracellular formate concentration at half-maximal flux was determined to be 900 microM.(ABSTRACT TRUNCATED AT 250 WORDS)

L11 ANSWER 29 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 17
ACCESSION NUMBER: 1994:460233 CAPLUS
DOCUMENT NUMBER: 121:60233
TITLE: 13C NMR Spin-lattice relaxation study of carbonyl carbon-water interaction in the Aerosol OT reversed micelles
AUTHOR(S): Yoshino, Akihiro; Okabayashi, Hirofumi; Yoshida, Tadayoshi
CORPORATE SOURCE: Department of Applied Chemistry, Nagoya Institute of Technology, Nagoya, 466, Japan
SOURCE: Journal of Physical Chemistry (1994), 98(28), 7036-40
CODEN: JPCHAX; ISSN: 0022-3654
DOCUMENT TYPE: Journal
LANGUAGE: English
AB For Aerosol OT (I) reversed micelle systems in dodecane, heptane, and benzene, the effect of solubilized H2O and D2O on the 13C NMR spin-lattice relaxation for the two carbonyl carbons of a I mol. was investigated in connection with I-water interaction. The contribution of water mols. to the observed spin-lattice relaxation rate was calculated The carbonyl group of the α-chain was more tightly bound to water mols. than that of the β-chain. The difference in an interaction between the carbonyl group and water mols. was reflected in the 13C chemical shift variation of the two carbonyl carbons.

L11 ANSWER 30 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 18
ACCESSION NUMBER: 1994:466330 CAPLUS
DOCUMENT NUMBER: 121:66330
TITLE: Self-Diffusion of Surfactants, Hydrocarbons, and Water in an L1 Phase and a Cubic Phase. Influence of Surfactant and Hydrocarbon Chain Lengths
AUTHOR(S): Panitz, J.-C.; Gradzielski, M.; Hoffmann, H.; Wokaun, A.
CORPORATE SOURCE: Physical Chemistry, University of Bayreuth, Bayreuth, D-95440, Germany
SOURCE: Journal of Physical Chemistry (1994), 98(27), 6812-17
CODEN: JPCHAX; ISSN: 0022-3654
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The pulsed field gradient NMR method has been used to determine self-diffusion coeffs. of surfactant mols., solubilized hydrocarbons, and D2O solvent in ternary N-alkyl-N,N-dimethylamine oxide/alkane/D2O surfactant systems. In the micellar phase, diffusion is governed by hydrodynamic transport of the micelles, supplemented by an exchange of solubilized hydrocarbon upon micellar collisions. This model is tested by variations in both the surfactant chain length and in the size of the hydrocarbon mols. In the cubic ("ringing gel") phase, the solvent still exhibits values of the diffusion coeffs. that are typical for motion in a continuous water phase, with the microemulsion droplets acting as obstacles. Mobilities of the surfactant in the gel state are low and have been determined only for the

surfactant with the shortest chain length (C12DMAO). Exchange of hydrocarbon between micellar entities in the gel occurs by a hopping process; the associated rate decreases with the surfactant chain length. The latter process is restricted to domains with sizes on the order of a few microns.

L11 ANSWER 31 OF 51 SCISEARCH COPYRIGHT (c) 2007 The Thomson Corporation on STN

ACCESSION NUMBER: 1994:359836 SCISEARCH
THE GENUINE ARTICLE: NQ723
TITLE: METAL-ASSISTED RACEMIZATION OF THE ATROPISOMERS OF A 1,1'-BINAPHTHYL SKELETON VIA A SYN TRANSITION-STATE
AUTHOR: ASHBY M T (Reprint); GOVINDAN G N; GRAFTON A K
CORPORATE SOURCE: UNIV OKLAHOMA, DEPT CHEM & BIOCHEM, NORMAN, OK 73019 (Reprint)
COUNTRY OF AUTHOR: USA
SOURCE: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, (1 JUN 1994) Vol. 116, No. 11, pp. 4801-4809. ISSN: 0002-7863.
PUBLISHER: AMER CHEMICAL SOC, 1155 16TH ST, NW, WASHINGTON, DC 20036 USA.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 44
ENTRY DATE: Entered STN: 1994
Last Updated on STN: 1994

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Delta/lambda-(delta/lambda-1,1'-Biisoquinoline)bis(2,2'-bipyridine)ruthenium(II) bis(hexafluorophosphate) (2) exists as an similar to 3:1 mixture of its two diastereomeric forms in acetone solutions at 25 degrees C. The major isomer, (Delta,delta/Delta lambda)-2, crystallizes in the monoclinic space group C2/c with Z = 8, a = 29.12(1), b = 18.593(7), and c = 17.85(1) Angstrom, beta = 127.81(4)degrees, R = 0.053, and R(W) = 0.062 at 25 degrees C. As expected, the 1,1'-biisoquinoline ligand is nonplanar, which is a result of a transannular steric interaction between H-8 and H-8'. Diastereomerically pure samples of 2 were found to isomerize rapidly in solution at room temperature in the absence of light to give a thermodynamic mixture of the two diastereomers. The rate data for the latter equilibrium at 80 degrees C are K = 2.89, k(6a(maj)-->6a(min)) = 12.7(3) s(-1), and k(6a,(min)-->6a(maj)) = 36.6(9) s(-1). The activation parameters were determined in the temperature range of 50-90 degrees C: Delta H-double dagger (maj-->min) = 68.7 kJ mol(-1), Delta S-double dagger(maj-->min) = -21 J K-1 mol(-1), Delta H-double dagger(min-maj) = 66.1 kJ mol(-1), and Delta S-double dagger(min-->maj) = -38 J K-1 mol(-1). Spin saturation transfer (SST), spin inversion transfer (SIT), and two-dimensional exchange spectroscopy (2D EXSY) NMR experiments using 2 and its 2,2'-bipyridine-d(8) analogue demonstrate that the interconversion of the two diastereomers is the result of an intramolecular process of C-2 symmetry that does not change the cis/trans relationship between the 1,1'-biisoquinoline and 2,2'-bipyridine ligands. Irregular mechanisms that involve breaking just one of the ruthenium-isoquinoline bonds have been ruled out because the rate of isomerization of a water-soluble derivative of 2, Delta/lambda-(delta/lambda-1,1'-biisoquinoline) bis(2,2'-bipyridine)ruthenium(II) dichloride, is essentially the same in D2O containing 1 M LiCl (k(6a(maj)-6a(min)) = 5.7(2) s(-1)) and 1 M DCl (k(6a(maj)-->6a(min)) = 7.1(1) s(-1)) at 80 degrees C. We therefore conclude that interconversion of the two diastereoisomers of 2 takes place by a regular mechanism that involves atropisomerization of the eta(2)-1,1'-biisoquinoline ligand via a syn transition state.

L11 ANSWER 32 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:515423 CAPLUS

DOCUMENT NUMBER: 123:66594
TITLE: Solubilization in micellar solutions and phase diagram of microemulsion formation for cationic surfactant
AUTHOR(S): Li, Ganzuo; Hao, Shuxuan; Li, Ying; Song, Lianghan; Fan, Aihu
CORPORATE SOURCE: Dep. Chem., Shandong Univ., Jinan, Peop. Rep. China
SOURCE: Shandong Daxue Xuebao, Ziran Kexueban (1994), 29(4), 437-44
CODEN: SDXKEU; ISSN: 0559-7234
PUBLISHER: Shandong Daxue
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB The effect of various kinds of alcs. on the forming of microemulsions in CTAB/H2O/octane/alc. systems was studied. While the mol. wts. of alcs. were changed, from investigating the pseudoternary phase diagrams, laws about the variation of the kinds and areas of microemulsions with alc. mol. wts. have been gotten. And NMR method was used to determine the solubilizated location of benzyl alc. (or m-dimethyl benzene) in CTAB/D2O micellar system, and the former laws were verified.

L11 ANSWER 33 OF 51 MEDLINE on STN
ACCESSION NUMBER: 1998044626 MEDLINE
DOCUMENT NUMBER: PubMed ID: 9383378
TITLE: Conformation of a water-soluble derivative of taxol in water by 2D-NMR spectroscopy.
AUTHOR: Gomez Paloma L; Guy R K; Wrasidlo W; Nicolaou K C
CORPORATE SOURCE: Department of Chemistry, Scripps Research Institute, La Jolla, CA 92037, USA.
SOURCE: Chemistry & biology, (1994 Oct) Vol. 1, No. 2, pp. 107-12.
Journal code: 9500160. ISSN: 1074-5521.
PUB. COUNTRY: ENGLAND: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
(RESEARCH SUPPORT, U.S. GOV'T, NON-P.H.S.)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199801
ENTRY DATE: Entered STN: 29 Jan 1998
Last Updated on STN: 29 Jan 1998
Entered Medline: 13 Jan 1998

AB BACKGROUND: Taxol is a natural product produced by the Pacific yew, Taxus brevifolia, that has emerged as a prominent chemotherapeutic agent for the treatment of solid tumors. It binds to microtubules, stabilizing them and arresting cells in mitosis. Taxol has been produced synthetically and a wealth of structure-activity data has recently emerged. To data, however, no single conformational model exists for the interpretation of these data. Studies of taxol and its analogs in organic solvents showed two distinct conformations, one in which the 3'-benzamido group and the 2-benzoyl group are in close proximity, and another in which the 2-benzoyl group is instead close to the 3'-phenyl group. We decided to use a derivative of taxol that has improved water-solubility to determine the structure of taxol in water. RESULTS: We have synthesized and characterized a stable water-soluble derivative of taxol that binds to microtubules and has a cytotoxicity profile very similar to that of taxol. 1D and 2D 1H NMR experiments with this bioactive compound in D2O indicate the presence of one conformer with a well-defined structure. In this structure, the 2-benzoyl group is clustered with the 3'-phenyl group. CONCLUSION: The determination of the conformation of taxol in water may allow quantitative three-dimensional interpretation of the structure-activity data obtained for taxol, and hence enable the design of novel taxol mimics.

L11 ANSWER 34 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 1991-322089 [44] WPIDS

DOC. NO. CPI: C1991-139289 [21]
TITLE: New substance WF-19849 from kernia sp. - has antifungal activity against e.g. candida albicans
DERWENT CLASS: B04; C03; D16
INVENTOR: FUJIE A; IWAMOTO T; NITTA K; OKUHARA M; SHIGEMATSU S
PATENT ASSIGNEE: (FUJI-C) FUJISAWA PHARM CO LTD
COUNTRY COUNT: 1

PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 03216192	A	19910924	(199144)*	JA		

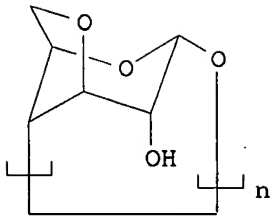
APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 03216192	A	JP 1990-9196	19900117

PRIORITY APPLN. INFO: JP 1990-9196 19900117
AN 1991-322089 [44] WPIDS
AB JP 03216192 A UPAB: 20050502
(1) Substance WF-19849 and its salts that have physico-chemical properties of (1) colour and nature ; white powder (2) m.pt 218 - 229 deg C (decompose) (3) spec. rotation alpha D = +54.1 deg C (C = 1.0, H2O), (4) mol. formula ; C18H23N7O5, (5) Mass (FARMS) ; 394 (M+H) +, (6) UV lamda max H2O = 260 nm, lambda max H2O+0.01NHCl = 258 nm lambda max H2O+0.01N NaOH = 260 nm, (7) IR ; max KBr = 3330, 3180, 2960, 1635, 1595, 1470, 1385, 1325, 1290, 1240, 1205, 1168, 1065, 955, 820, 795, 715, 640 cm-1, (8) 1H-NMR delta (D2O),(9) 13C-NMR (D2O) (10) solubility ; easily soluble (H2O), slightly soluble (MeOH, EtOH)M insol. (CHCl3, EtOAc). (11) colour reaction ; positive (Cs(SO4)2, Ninhydrin), (12) thin layer chromatography; Rf=0.6 (silica gel (Kiesel gel 60F - 254), developer (isopropanol : H2O = 7 : 3). Rf = 0.3. (silica gel (ibid), developer (n-buOH : AcOH : H2O = 4 : 1 : 2) and (13) basicity; amphoteric (2) Prepn for substance WF-19849 by culturing the substance WF-19849 producing Kernia sp., next by collecting it from the culture.

USE/ADVANTAGE - Substance WF-19849 has antifungal effect e.g. Candida albicans, it is expected for an antifungal drug.

L11 ANSWER 35 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:680410 CAPLUS
DOCUMENT NUMBER: 115:280410
TITLE: Per-3,6-anhydro-α-cyclodextrin and per-3,6-anhydro-β-cyclodextrin
AUTHOR(S): Ashton, Peter R.; Ellwood, Paul; Staton, Ian; Stoddart, J. Fraser
CORPORATE SOURCE: Dep. Chem., Univ. Sheffield, Sheffield, S3 7HF, UK
SOURCE: Journal of Organic Chemistry (1991), 56(26), 7274-80
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB The synthesis of the per-3,6-anhydro derivs., e.g. I (n = 6, 7) of α- and β-cyclodextrins (CDs) is described starting from the corresponding per-6-O-tosylates. These could only be obtained as pure compds. following repeated HPLC under reversed phase conditions of the crude products isolated after tosylation of α-CD and β-CD in pyridine with p-toluenesulfonyl chloride. Treatment of the per-6-O-tosyl-α- and β-CDs with warm aqueous NaOH solns. (50-60 °C) afforded the per-3,6-anhydro-α- and β-CDs in good yields. The development of an alternative and successful strategy for the synthesis of per-3,6-anhydro-α-CD from the known per-2,3-di-O-benzoyl-6-tosyl-α-CD relies upon the use of Et3N as base in refluxing aqueous MeOH. The per-3,6-anhydro-CDs have been fully characterized by FABMS and NMR spectroscopy. Their specific optical rotations, which are solvent dependent, confirm the chiral nature of these mols. The anhydrides are soluble in such widely different solvents as CH2Cl2 and H2O. There is evidence from FABMS that per-3,6-anhydro-α-CD forms a complex with the triethylammonium cation while per-3,6-anhydro-β-CD solubilizes PhNO2 in D2O solns.

L11 ANSWER 36 OF 51 BIOSIS COPYRIGHT (c) 2007 The Thomson Corporation on STN DUPLICATE 19

ACCESSION NUMBER: 1992:102964 BIOSIS
DOCUMENT NUMBER: PREV199293059514; BA93:59514
TITLE: SOLUBILITY OF DOMOIC ACID IN WATER AND IN NON-AQUEOUS SOLVENTS.
AUTHOR(S): FALK M [Reprint author]; SETO P F; WALTER J A
CORPORATE SOURCE: INST MARINE BIOSCI, NATIONAL RESEARCH COUNCIL CANADA, 1411 OXFORD ST, HALIFAX, NS B3H 3Z1, CAN
SOURCE: Canadian Journal of Chemistry, (1991) Vol. 69, No. 11, pp. 1740-1744.
CODEN: CJCHAG. ISSN: 0008-4042.
DOCUMENT TYPE: Article
FILE SEGMENT: BA
LANGUAGE: ENGLISH
ENTRY DATE: Entered STN: 12 Feb 1992
Last Updated on STN: 13 Feb 1992

AB The solubility of domoic acid (DA) in H2O and D2O, in aqueous NaCl solution and in several non-aqueous solvents was measured by NMR and UV spectroscopies. The solubility in water is comparable with that of aminoacids such as glutamic acid and aspartic acid. It is markedly pH-dependent, passing through a minimum at the isoelectric point, the increase towards both higher and lower pH values indicating that the anionic and cationic forms are more soluble than the neutral form. The effect of NaCl on the solubility of DA in water is negligible. The solubility of DA in alcohols is lower than in water but it is much higher than the solubility of glutamic acid or aspartic acid. The octanol-water partition coefficient for DA at pH 5.32, Kow=0.0037, was obtained by a direct UV measurement. The low value of Kow indicates that aquatic organisms cannot take up DA directly from the water and bioaccumulation may proceed only through dietary intake.

L11 ANSWER 37 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 1988-238172 [34] WPIDS
DOC. NO. CPI: C1988-106655 [21]
TITLE: New antibiotic TAN-390 used to treat infection and in detergent - comprises (di:sodium) epoxy:propyl-adenosine-5-di:phosphate prepared by culturing Pseudomonas
DERWENT CLASS: B04; D16
INVENTOR: HARADA S; ONO H; TSUBOYA S
PATENT ASSIGNEE: (TAKE-C) TAKEDA CHEM IND LTD
COUNTRY COUNT: 1

PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 63170395	A	19880714	(198834)*	JA	9[0]	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 63170395	A	JP 1986-164403	19860712
JP 63170395	A	JP 1987-128964	19870525

PRIORITY APPLN. INFO: JP 1987-128964 19870525
AN 1988-238172 [34] WPIDS
AB JP 63170395 A UPAB: 20050429
New antibiotic TAN-930 and its disodium salt of formula (I) are new. Pseudomonas sp. microbe which cna produce antibiotic TAN-930, is cultured on medium, the TAN-390 is collected.
Pref. microbe is Pseudomonas sp. PK-5 (FERM P-8832, IFO-14515). The physicochemical properties of (I) are (1) nature; white solid, (2) spec. rotation; (alpha)23D-26 deg.+/- 10 deg. (C = 0.51, H2O), (3) elemental analysis (%); C 28.63, H 3.93, N 12.96, P 11.56, Na 7.2. (Calculated as 2 mol. of H2O is contained),(4) n.w.; m/z 512 (M+H)+ by SI-MS, (5) molecular formula; C13H17N5O10P2Na2, (6) UV; H2O, lambda max 258 +/- 3nm (E(1%)1cm = 295 +/- 50), (7) IR (KBr); 3400, 1650, 1610, 1580, 1480, 1420, 1380, 1340, 1240, 1110, 1080, 940, 830, 800, 730, 650, 510 (cm(-1)), (8) 13C-NMR; 100M H2D2O, (9) solubility; soluble in H2O, DMSO, insol. in EtOAc, acetone, CHCl3, (10) colour reaction position in periodic acid-bentidine ammonium molybdate-perchloric acid, KMNO4, negative in ninhydrin, Sakaguchi, Barton, (11) TLC cellulose f; acetonitrile:H2O (4:1) Rf = 0.08, buOH:AcOH:H2O (2:1:1) Rf = 0.31, (12) HPLC; (YMC-PAK A312, 6% meOH/0.01M phosphate buffer 8pH 6.3), flow rate 2 ml/min), Rt = 4.8 min, (13) category of the substance; neutral, (14) 1HNMR, (400 MHz, D2O).

USE/ADVANTAGE - (I) has antibacterial effect against Gram positive and negative bacteria. It can be used for treatment of infection by oral or parenteral administration to human or other animals and it is also useful in detergent. Pref. daily dose is 5-20 mg/kg (p.c., i.m.), 5-50 mg/kg (p.o.).

L11 ANSWER 38 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 1987-046450 [07] WPIDS
DOC. NO. CPI: C1987-019338 [21]
TITLE: New antibiotic tokimycin - obtd. by culturing streptomyces genus of actinomyces
DERWENT CLASS: B04; D16
INVENTOR: TANAKA N
PATENT ASSIGNEE: (BANY-C) BANYU PHARM CO LTD
COUNTRY COUNT: 1

PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 62003789	A	19870109	(198707)*	JA	9[0]	
JP 05071234	B	19931006	(199343)	JA	9	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 62003789	A	JP 1985-141554	19850629
JP 05071234	B	JP 1985-141554	19850629

FILING DETAILS:

PATENT NO	KIND		PATENT NO
JP 05071234	B	Based on	JP 62003789 A

PRIORITY APPLN. INFO: JP 1985-141554 19850629
AN 1987-046450 [07] WPIDS
AB JP 62003789 A UPAB: 20050424
Antibiotic Tokimycin A and its pharmaceutically tolerable salts are new and have properties (a) Analysis (%) : C, 58.3; H, 61; N, 2.3 ; 0.33.5; (b) Mol. formula is C29H37NO11 and mol.weight = 574 ; (c) M.pt. of Tokimycin A hydrochloride = 106 - 112 deg.C; (d) Infrared adsorption spectra is given; (e) Ultraviolet absorption spectra is given with as follows: in 0.1 N hydrochloric acid aqueous solution lambda maximum (E1% 1 cm) = 268 (90), 285 (sh), 525 (435) in water lambda maximum (E1% 1 cm) = 215 (333), 254 (137), 435 (355); (f) 1H-NMR Spectra (400 Mhz, D2O) is given; (g) Deg. of specific rotation of Tokimycin A is (alpha)22.5 D = -50.0 deg. (C=0.098, B2O); (h) Colouration reaction on Tokimycin A hydrochloride is: Magnesium acetate positive Nitropluside-acetaldehyde positive Dragendorf positive Ninhydrin negative Erson. Morgan negative; (i) Tokimycin A hydrochloride is soluble in water, methanol or ethanol, and insol. in acetone, ethyl acetate, chloroform or hexane (j) Tokimycin A hydrochloride is hygroscopic or crystalline powder. Basic.
Antibiotic Tokimycin A is produced by culturing antibiotics Tokimycin A - producing actinomycetes of Streptomyces genus in culture medium containing nutrient source in aerophilic conduction to yield and accumulate Tokimycin A and removed obtd. Tokimycin A.
Streptomyces genus of actinomycetes is e.g. Streptomyces virginiae IM 7923 strain FERM P 8321.
USE - Naphthoquinone series of antibiotics have antibiotic property useful in pharmaceuticals.

Member(0002)
ABEQ JP 93071234 B UPAB 20050424
Antibiotic Tokimycin A and its pharmaceutically tolerable salts are new and have properties of (a) Analysis (%) : C, 58:3; H, 61; N, 2.3; 0.35.5; (b) Mol. formula is C29H37NO11 and molecular wt. is 574; (c) M.pt. of Tokimycin A hydrochloride is 106 - 112 deg.C; (d) Infrared adsorption spectra is given; (e) Ultraviolet absorption spectra is given with as follows: in 0.1 N hydrochloric acid aq. soln. lambda max. (E1% 1 cm) = 268 (90), 285 (sh), 525 (435) in water lambda max. (E1% 1 cm) = 215 (333), 254 (137), 435 (355); (f) 1H-NMR Spectra (400 Mhz, D2O) is given; (g) Deg. of specific rotation of Tokimycin A is (alpha)22.5 D = -50.0 deg (C=0.098, B2O); (h) Colouration reaction on Tokimycin A hydrochloride is: Magnesium acetate positive Nitropluside-acetaldehyde position Dragendorf positive Ninhydrin negative Erson. Morgan negative; (i) Tokimycin A hydrochloride is soluble in water, methanol or

ethanol, and insol. in acetone, ethyl acetate, chloroform or hexane; (j) Tokimycin A hydrochloride is hygroscopic or crystalline powder. Basic. Antibiotic Tokimycin A is produced by culturing antibiotics Tokimycin A - producing actinomycetes of Streptomyces genus in culture medium contg. nutrient source in aerophillic conduction to yield and accumulate Tokimycin A and removed obtd. Tokimycin A. Streptomyces genus of actinomycetes is e.g. Streptomyces virginiae IM 7923 strain FERM P 8321.

USE - Naphthoquinone series of antibiotics have antibiotic property useful in pharmaceuticals. (J62003789-A)

L11 ANSWER 39 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 1987-031714 [05] WPIDS
DOC. NO. CPI: C1987-013349 [21]
TITLE: G0069C carcinostatic and antifungal cpd. production - by culturing Streptomyces strain in liquid medium in aerobic conditions
DERWENT CLASS: B02; C02; D16
INVENTOR: DEN K; ISHIDA N; KAJITANI A; MARUNAKA T; MINAMI Y; MIYAKE Y; SEKI C
PATENT ASSIGNEE: (TAIH-C) TAIHO PHARM CO LTD
COUNTRY COUNT: 1

PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 61268685	A	19861128	(198705)*	JA	6[0]	
JP 03065360	B	19911011	(199145)	JA		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 61268685	A	JP 1985-110779	19850523
JP 03065360	B	JP 1985-110779	19850523

PRIORITY APPLN. INFO: JP 1985-110779 19850523
AN 1987-031714 [05] WPIDS
AB JP 61268685 A UPAB: 20050629
G0069C and its salts are of formula (I).
G0069C has the following physico-chemical properties (1) Mol.weight: 287 (from FAB MS) (2) Soluble in water; hardly soluble in ether and chloroform. (3) IR-absorption spectrum. Maximum at 3350, 1770, 1670, 1630, 1390, 1350, 1135, 1055 cm-1 (4) proton -NMR spectrum (D2O) has peaks centred at (ppm) 1.58, 3.40, 3.86, 4.48, (5) No intense absorption between 220 nm and 350 nm. G0069C is produced by culture of a G0069C-producing bacterium of Streptomyces (e.g. Streptomyces brunneogriseus Furuma: et Okuda subsp. bannaensis G0069 (FERM 706)) in a liquid medium under aerobic condition.

USE/ADVANTAGE - G0069C has carcinostatic and antifungal activity and is useful for a medicine.

L11 ANSWER 40 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1986:105405 CAPLUS
DOCUMENT NUMBER: 104:105405
TITLE: Hydrogen exchange in the hydrophilic regions of detergent-solubilized M13 coat protein detected by carbon-13 nuclear magnetic resonance isotope shifts
AUTHOR(S): Henry, Gillian D.; O'Neil, Joe D. J.; Weiner, Joel H.; Sykes, Brian D.
CORPORATE SOURCE: Dep. Biochem., Univ. Alberta, Edmonton, AB, T6G 2H7, Can.
SOURCE: Biophysical Journal (1986), 49(1), 329-31

CODEN: BIOJAU; ISSN: 0006-3495
DOCUMENT TYPE: Journal
LANGUAGE: English
AB M13 coat protein was selectively labeled at the carbonyl C of lysine, proline, or phenylalanine by inclusion of the appropriate 13C-enriched amino acid in the culture medium. After solubilization with SDS, 13C NMR spectra were recorded in D2O. Chemical shift changes which were pH-dependent were recorded. The pH values at which the collapse of the splitting occurs corresponded to a rate of 40/s, which was related to a freely exposed peptide N-H by an equation. All amide hydrogens exchanged at slower rates than those observed for a small peptide (Hawkes, G. E. et al., 1978).

L11 ANSWER 41 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:157378 CAPLUS
DOCUMENT NUMBER: 100:157378
TITLE: Mechanisms of polymer-supported catalysis. 5. Solvation of quaternary onium ions in polystyrene gels by carbon-13 NMR spectroscopy
AUTHOR(S): Ford, Warren T.
CORPORATE SOURCE: Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA
SOURCE: Journal of Polymer Science, Polymer Chemistry Edition (1984), 22(3), 509-18
CODEN: JPLCAT; ISSN: 0449-296X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 13C-NMR linewidths and spin-lattice relaxation times were determined for soluble and crosslinked polystyrenes containing quaternary phosphonium and ammonium ions. Solubilities and NMR linewidths show that the solvating abilities toward tributylphosphonium ions are CDCl3 [865-49-6] > MeOH [67-56-1] > D2O > C6H6 [71-43-2] > PhMe [108-88-3]; toward trimethylammonium ions, MeOH > CDCl3 > D2O > PhMe; and toward the nonpolar polymer backbone, CDCl3 > C6H6 > PhMe > MeOH > D2O.

L11 ANSWER 42 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 1983-714080 [29] WPIDS
DOC. NO. CPI: C1983-067879 [21]
TITLE: Antibiotic KA-6643-J - obtd. by fermentation using suitable streptomyces strains
DERWENT CLASS: B04; D16
INVENTOR: ITOU H; IWASAKI A; KIMURA S; MIZOGUCHI T; MORI T; MURAKAMI A; NAKAYAMA M; OGUCHI M; TANABE S
PATENT ASSIGNEE: (KOWA-C) KOWA CO LTD
COUNTRY COUNT: 1

PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 58098090	A	19830610	(198329)*	JA	8	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 58098090	A	JP 1981-194888	19811203

AN 1983-714080 [29] WPIDS
AB JP 58098090 A UPAB: 20050421
Antibiotic KA-6643-J and its salts and esters are new, of which the Na salt has the following properties: (1) Appearance: colourless powder. (2)

Elemental analysis: C 35.4 +- 0.5, H 4.0 +- 0.5, N 5.5 +- 0.5, S 13.0 +- 1.0, Na 9.5 +- 1.0. (3) Mol. weight 440-490. (4) UV: (in water), maximum absorption at 285 nm. (5) IR: (KBr), major peak at 1770 cm-1. (6) 1H-NMR: (D2O, 200 MHz, the major peaks from HOD 4.9 ppm.
located at 1.61 ppm. (s, 3H), 1.69 ppm. (s, 3H), 2.00 ppm. (2, 3H). (7) TLC: on cellulose plate, Rf is 0.23 (n-BuOH/i-PrOH/water (7:7:6)); Rf is 0.60 (EtOH/water (7:3)). (8) HPLC: column: Radial pack A (RTM) (0.8 x 10 cm.), solvent: 11% MeOH/0.05M KH2PO4, flow rate: 1.0 ml/ min., retention time: 5.1 min. (9) Solubility: soluble in water and
water, insoluble in EtOAc and CHCl3. (10) Colour reaction: positive to Ehrlich, negative to ninhydrin.
KA-6643-J has the following MIC values (mcg/ml): Staphylococcus aureus 209P JC-1, 6.25 (mcg/ml.); Bacillus subtilis ATCC 6633; 6.25; Escherichia coli NIHJ JC-2, 1.56; Klebsiellapneumoniae PCI602, 6.25; Enterobacter cloacae IID977, 6.25; Proteus vulgaris IID874, 0.78; Serratia marcescens NHL, 6.25; Salmonella typhi H-901, 1.56; Pseudomonas aeruginosa NCTC 10490, 6.25. KA-6643-J has beta-lactamase inhibiting activity.
KA-6643-J is produced by Streptomyces sp. KC-6643 together with KA-6643-A, KA-6643-B, KA-6643-D, and KA-6643-F.

L11 ANSWER 43 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1983:477369 CAPLUS
DOCUMENT NUMBER: 99:77369
TITLE: A comparative study of micellar solubilization for combinations of surfactants and solubilizates using the Fourier transform pulsed-gradient spin-echo NMR multicomponent self-diffusion technique
AUTHOR(S): Stilbs, Peter
CORPORATE SOURCE: Inst. Phys. Chem., Uppsala Univ., Uppsala, S-751 21, Swed.
SOURCE: Journal of Colloid and Interface Science (1983), 94(2), 463-9
CODEN: JCISA5; ISSN: 0021-9797
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The degree of solubilization for all combinations of 6 surfactants (Na dodecanoate, Na dodecyl sulfate, Na octylbenzene sulfonate, Na phenylundecanoate, dodecyltrimethylammonium bromide, and dodecylhexaethyleneglycolmonoether) and 12 solubilizates (1-pentanol, 2-pentanol, 3-pentanol, tert-pentanol, methyl-Pr ketone, di-Et ketone, benzene, benzyl alc., crown 18-6, crown 12-4, 1,4-dioxane, and Et glycol) was determined at a surfactant concentration of 50 mg/mL D2O solution and low total solubilizate/surfactant ratios. The most striking observations concern the solubilization behavior of the nonionic surfactant; with the aliphatic type it solubilizates weakly, with aroms. as strongly as the other surfactants, and with crown ethers hardly at all. With the exception that dodecyltrimethylammonium bromide micelles solubilize ketones more weakly in a relative sense, the remaining 5 surfactants exhibit very similar solubilization characteristics. NMR-based evidence with regard to the site of solubilization of aroms. is discussed.

L11 ANSWER 44 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1982:412262 CAPLUS
DOCUMENT NUMBER: 97:12262
TITLE: Fourier transform NMR pulsed-gradient spin-echo (FT-PGSE) self-diffusion measurements of solubilization equilibriums in SDS solutions
AUTHOR(S): Stilbs, Peter
CORPORATE SOURCE: Inst. Phys. Chem., Uppsala Univ., Uppsala, S-751 21, Swed.
SOURCE: Journal of Colloid and Interface Science (1982), 87(2), 385-94

CODEN: JCISA5; ISSN: 0021-9797
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Solubilization equilibrium for homologous series of alcs., Me ketones, aroms., and crown ethers with Na dodecyl sulfate(SDS) micelles in D2O solution at 25°C were determined The degree of solubilization increases strongly with the number of carbon atoms in the solubilizate alkyl chains, corresponding to an increment in the standard free energy for transfer of solubilizate mols. from the aqueous to the micellar phase (ΔGp0) of .apprx. -2.6 kJ mol-1 for each -CH2- group. Hydrocarbon chain branching in the solubilizate mols. decreases the degree of solubilization, as compared to conditions for alkyl compds. Crown ether solubilization increases strongly with ring size. Comparative studies with lauryltrimethylammonium bromide micelles do not show this trend, suggesting that the effect can be ascribed to the Na binding capability of the larger crown ethers, and that crown ethers are solubilized at the SDS micellar surface.

L11 ANSWER 45 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 1980-45569C [26] WPIDS
TITLE: Antimicrobials active on plant pathogens and Gram negative bacteria - contain TAI-A as active ingredients
DERWENT CLASS: B04; C03; D16
INVENTOR: HARA H; KAMIGOORI K; MORI E; NAGATE T; NAMIKI S; OMURA S; SUGITA K
PATENT ASSIGNEE: (TAIS-C) TAISHO PHARM CO LTD
COUNTRY COUNT: 1

PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 55064509	A	19800515	(198026)*	JA		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 55064509	A	JP 1978-138672	19781110

AN 1980-45569C [26] WPIDS
AB JP 55064509 A UPAB: 20050418
Antimicrobial agents contain as effective ingredient TAI-A having the following properties: (a) elemental analysis C 41.44%, H 6.27%, N 1.32%; (b) molecular weight 950-1050; (c) alpha D23 + 157.3 degrees (c = 0.5, water); (d) specific spectrum; (e) specific NMR spectrum (60 MHz, D2O); (f) solubility: soluble in H2O and DMSO; ins l. in MeOH, EtOH, CHCl3, Me2CO and pyridine; (g) colour reaction: positive to Molisch and anthrone reactions; the hydrolysate, positive to ninhydrin and Elson-Morgan's reactions; (h) pKa: 4.2 (in aqueous solution), basic; (i) appearance: white powder; (j) chromatography: Rf value- TLC (silica gel 60 F254, Merck & Co.) 0.40 (65% n-PrOH), 0.21 (n-BaOH:pyridine:H2O= 6:4:2.5), 0.18 (n-BuOH:EtOH:H2O= 3:2:2); paper chromatography (Toyo filter paper Number 50), 0.16 (65% n-PrOH), 0.42 (pyridine:n-PrOH:AcOH:H2O); (k) UV is no characteristic absorption at 210-360 nm (in 1% aqueous solution); (l) melting point: decomposing at 137-142 degrees C, no clear m.pt.
TAI-A is effective against plant pathogenes (e.g. Ophiobolus miyabeanus, Gibberella fujikuroi, Fusarium lycopersici, Botrytis cinerea, Fusarium oxysporum) and Gram-negative bacteria. The antimicrobial action is enhanced by addition of maltose, maltotriose, maltotetraose, maltopentaose, maltohexaose or maltoheptaose.

L11 ANSWER 46 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:507417 CAPLUS
DOCUMENT NUMBER: 89:107417
TITLE: Binding and photoionization of N-substituted 2-chlorophenothiazines in SDS micelles
AUTHOR(S): Iwaoka, Teiki; Kondo, Michio
CORPORATE SOURCE: Cent. Res. Lab., Sankyo Co., Ltd., Tokyo, Japan
SOURCE: Chemistry Letters (1978), (7), 731-4
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English
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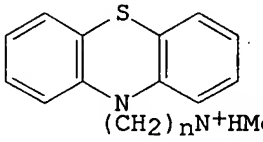

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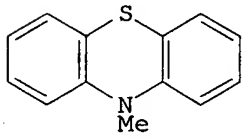

II

AB Chlorpromazine (I; n = 3) and its analogs I (n = 2, 6, 10) were prepared and their binding sites and photochem. reactions in the aqueous micelle of Na OSO2O(CH2)11Me were studied. Comparison of the NMR of I in dodecane, dioxane, EtOH, D2O, and in the stated micelle indicates that I are solubilized into the micelle, with the ammonium group exposed to the water phase. The same types (i.e., bleaching, sulfoxide formation, dehydrochlorination) of photochem. reactions occurred for I regardless of the value of n.

L11 ANSWER 47 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 1977-60452Y [34] WPIDS
TITLE: (7)-Methoxy cephalosporin antibiotic Y-G 19ZD3 - prepared by culturing Streptomyces organonensis Y-G19Z
DERWENT CLASS: B04; D16
INVENTOR: GUSHIMA H; MURAKAMI K; OKA Y; OSONO T; SAITO T; SASAKI T; TAKAHASHI I; WATANABE S; YAMAGUCHI Y
PATENT ASSIGNEE: (YAMA-C) YAMANOUCHI PHARM CO LTD
COUNTRY COUNT: 1

PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 52083702	A	19770712	(197734)*	JA		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 52083702	A	JP 1976-293	19760101

AN 1977-60452Y [34] WPIDS
AB JP 52083702 A UPAB: 20050417
7-Methoxycephalosporin antibiotic Y-G19ZD3 is new. It decomposes at 160-170 degrees C and is readily soluble in water, sparingly soluble in MeOH and EtOH, almost insoluble in other organic solvents. It is amphoteric, positive to ninhydrin reaction. UV:Amax 272 um (E1% 176; 1/100 M phosphate buffer of pH 6.4). IR:V max 1 cm (KBr) 3420,1765,1625,1520,1405,1220,1030,640 cm-1 NMR: (D2O)1.80, 2.43, 3.35-3.82, 3.47, 3.82, 4.01, 5.13 ppm.
(I) has potent antimicrobial action against gram negative bacteria, it is

effective against cephalosporing resistant strains, also useful as intermediate in preparation of cephalosporin cpds.
(I) is produced by culture of a new strain of Streptomyces organonensis Y-G19Z isolated from the soil of Oganocho, Chichibu-gun, Saitama Pref., Japan (FERM-P 2725; ATCC Number 31167).

L11 ANSWER 48 OF 51 WPIDS COPYRIGHT 2007 THE THOMSON CORP on STN
ACCESSION NUMBER: 1977-60451Y [34] WPIDS
TITLE: (7)-Methoxy cephalosporin antibiotic Y-G 19ZD2 - prepared by culturing Streptomyces organonensis Y-G19Z
DERWENT CLASS: B04; D16
INVENTOR: GUSHIMA H; MURAKAMI K; OKA Y; OSONO T; SAITO T; SASAKI T; TAKAHASHI I; WATANABE S; YAMAGUCHI Y
PATENT ASSIGNEE: (YAMA-C) YAMANOUCHI PHARM CO LTD
COUNTRY COUNT: 1

PATENT INFO ABBR.:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 52083701	A	19770712	(197734)*	JA		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 52083701	A	JP 1976-290	19760101

AN 1977-60451Y [34] WPIDS
AB JP 52083701 A UPAB: 20050417
7-Methoxycephalosporin antibiotic Y-G19ZD2 (I) is new. (I) turns brown at about 160 degrees C and decomposes at 165-172 degrees C.
It is readily soluble in water, sparingly soluble in MeOH and EtOH, almost insoluble in other organic solvents. It is amphoteric, positive to ninhydrin reaction. UV: Amax (water) 275 mu (E1% 160) IR: V max (KBr) 3420,1765,1625,1520,1405,1225,1025,630 cm-1. NMR: (D2O) 1.87,2.41, 3.24-3.77, 3.42, 3.73-4.21, 3.92, 5.06 ppm. Paper chromatography: Whatman 1, developed by n-BuOH:AcOH:water (4:1:2 by volume) for 24 hr.(descending), the spot moves by 13 cm from the starting point. TLC: on fine crystalline cellulose, Rf value-0.37 (i-PrOH:AcOH:n-BuOH:water = 21:7:3:9), 0.43(n-PrOH:pyridine:AcOH:water=5:1:0.3:3.9), 0.44(i-ProH:water =7:3).
(I) is mainly effective against gram negative bacteria. It is produced by culturing a new strain of Streptomyces Organonensis Y-G19Z isolated from the soil of Organo-cho, Chichibugun, Saitama Pref., Japan (FERM-P 2725; ATCC Number 31167). The organism is cultured under submerged aerobic conditions at 18-35 pref. 30 degrees C, and pH 5-10, especially 6-8, for 3-10 days.

L11 ANSWER 49 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:198213 CAPLUS
DOCUMENT NUMBER: 86:198213
TITLE: Deuterium and nitrogen-14 NMR studies of amphiphilic liquid crystals. Effect of solubilization, electrolyte and temperature on water orientation
AUTHOR(S): Persson, Nils Ola; Lindman, Bjorn
CORPORATE SOURCE: Div. Phys. Chem. 2, Chem. Cent., Lund, Swed.
SOURCE: Molecular Crystals and Liquid Crystals (1977), 38(1-4), 327-44
CODEN: MCLCA5; ISSN: 0026-8941
DOCUMENT TYPE: Journal
LANGUAGE: English

AB D NMR on hexagonal and lamellar amphiphile-D2O mesophases was used to study the partial orientation of the water mols. and how the degree of orientation is influenced by solubilization of organic compds., by addition of simple electrolytes and by temperature changes.

Solubilization effects follow roughly the polarity of the solubilizate, a more polar solubilizate producing a greater reduction in the degree of water orientation, but important differences exist between-CO2- and -OSO3- end-groups of the surfactant. These results are discussed in terms of changes in amphiphile hydration and altered packing conditions in the aggregates. The effect of electrolyte addition depends markedly on both counterion and co-ion and is discussed on the basis of ion hydration. For Me4N octanoate-D2O system, the degree of water orientation increases with increasing water content, and this may arise from a particular counterion binding mechanism in this case. The counterion binding in this system as well as the NH4 octanoate-D2O system was further studied by means of 14N quadrupole splittings.

L11 ANSWER 50 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1973:446518 CAPLUS
DOCUMENT NUMBER: 79:46518
TITLE: Proton and deuteron magnetic resonance studies of lamellar lyotropic mesophases
AUTHOR(S): Johansson, Ake; Drakenberg, Torbjorn
CORPORATE SOURCE: Div. Phys. Chem., Lund Inst. Technol., Lund, Swed.
SOURCE: Liquid Cryst., Int. Liquid Cryst. Conf., [Pap.], 3rd (1972), Meeting Date 1970, Volume 1, 415-40. Editor(s): Brown, Glenn H. Gordon and Breach: London, Engl.
CODEN: 26UQAI
DOCUMENT TYPE: Conference
LANGUAGE: English
AB In the 2- and 3-component mesophases prepared from mixts. of D2O with n-octylamine (OA), OA.HCl, OA.HBr, cetyltrimethylammonium bromide, nonylphenol decaethylene glycol ether, nonylphenol hexaethylene glycol ether, n-octanoic acid, and n-decanol, the quadrupole splitting (Dv) observed in the deuteron NMR (DMR) originated from the anisotropic orientation of the elec. field gradients (EFG) experienced by the D+ of the D2O mols. The EFG anisotropy was due to partial orientation of the D2O mols. interacting with the hydrophilic groups of the amphiphile mols. The effects of concentration, temperature, and solubilization (e.g., of p-xylene) on the partial D2O orientation were evaluated by measuring the variations Δv. Exchange of D+ between D2O and the amphiphilic mols. was found. High-resolution PMR signals were observed in some mesophases. The alignment of some mesophases by a magnetic field (.apprx.14 kG) was observed by DMR and PMR.

L11 ANSWER 51 OF 51 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:132240 CAPLUS
DOCUMENT NUMBER: 80:132240
TITLE: NMR studies of the solubilization of aromatic compounds in sodium N-lauroyl sarcosinate solution
AUTHOR(S): Okabayashi, Hirofumi; Takahashi, Hitoshi; Okyuama, Masataka
CORPORATE SOURCE: Nagoya Inst. Technol., Nagoya, Japan
SOURCE: Nagoya Kogyo Daigaku Gakuho (1972), 24, 403-8
CODEN: NADGA8; ISSN: 0369-3171
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB Resonance line shifts of H atoms of sodium N-lauroylsarcosinate (I) were measured at several concns. of aromatic solubilizates in D2O. Benzene, p-xylene, mesitylene, and N,N-dimethylaniline

solubilized in I-D2O solution were adsorbed at the trans-N-Me of I mols. in the form of collision complexes, in addition to solubilization in the hydrocarbon part of I micelles. N-Methylaniline, PhNH2, and PhOH formed collision complexes with I. However, PhCO2H mols. were solubilized mainly in the hydrocarbon part near the peptide group of the micelles; there was some combination with the trans-N-Me group of I.

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     14:46:27 ON 16 JUL 2007
L1           190 SOLUB? (S) DEUTER? (S) WATER
L2           143 DUP REM L1 (47 DUPLICATES REMOVED)
L3            41 NMR AND L2
L4            45 PY>2001 AND L2
L5            98 L2 NOT L4
L6            21 L3 AND L5

     FILE 'STNGUIDE' ENTERED AT 14:58:32 ON 16 JUL 2007

     FILE 'MEDLINE, BIOSIS, CAPLUS, SCISEARCH, EMBASE, WPIDS' ENTERED AT
     14:59:37 ON 16 JUL 2007
L7           374 SOLUB? (S) D2O
L8           107 NMR AND L7
L9            32 PY>2001 AND L8
L10           75 L8 NOT L9
L11           51 DUP REM L10 (24 DUPLICATES REMOVED)

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